MAX-PLANCK-GESELLSCHAFT

GENNESYS
WHITE PAPER

A NEW EUROPEAN PARTNERSHIP
BETWEEN NANOMATERIALS SCIENCE & NANOTECHNOLOGY AND
SYNCHROTRON RADIATION AND NEUTRON FACILITIES

GENNESYS

GRAND
EUROPEAN INITIATIVE ON
NANOSCIENCE AND
NANOTECHNOLOGY

USING

NEUTRON- AND
SYNCHROTRON RADIATION
SOURCES

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EXECUTIVE

GENNESYS: A Responsible European Partnership between Nanomaterials Research Labs, Universities, Industry and the European Research Infrastructure

This GENNESYS strategy document is the result of an extensive European-wide study of the needs and opportunities for coordinating future research and development in nanomaterials science and nanotechnology for the advancement of technologies ranging from communication and information, health and medicine, future energy, environment and climate change to transport and cultural heritage. A further focus of this study has been the investigation of the future strategic role of the European research infrastructure, i.e. of the unique analytical potential provided by the European neutron and accelerator-based x-ray facilities in this effort. This study, carried out during 2003 – 2008, brought together leading European scientists and industrial specialists in the fields of materials science, physics, chemistry, biology, and engineering, as well as experts from the neutron and synchrotron radiation facilities. These experts headed thematic task forces with respect to particular research areas – such as information technology, catalysis or functional materials as well as energy and environment issues – and developed roadmaps through numerous informal seminars, workshops and discussion rounds involving colleagues across Europe and the world.

The key objectives of the GENNESYS task forces were:

- To assess the "state of the art" of nanoscience and technology in Europe;
- To identify future needs, opportunities and priorities in the field of nanomaterials science for solving urgent problems in Europe and around the world;
- To articulate fundamental scientific challenges, society needs and industrial potentials in this field;
- To define recommendations and objectives for future research, technologies, and development strategies which will lead to major advances;
- To pinpoint areas of research into nanomaterials science and technology that will most benefit from joint research strategies with synchrotron radiation and neutron facilities;
- To review and forecast the effects that a strategic use of large-scale facilities by nanomaterials scientists will have on the facilities;
- To provide evidence of the societal impact of the field and provide a forum for coordinated community-wide communications between basic researchers, industry, policy-makers and the public, respectively;
- To establish a strategic European research programme encapsulated "Nanomaterials research and technology for future technologies exploiting neutron and accelerator-based x-ray facilities".

The GENNESYS initiative was triggered by the fact that Europe's expertise in nanomaterials science is excellent (highlighted by many revolutionary discoveries during the last two decades) but fragmented into scientific disciplines, sectors and national (often regional) efforts which are – on an international scale – often subcritical; and that Europe would benefit considerably from a strategic pan-European, multi-disciplinary research involving all sectors and the most advanced European research infrastructure for the fine analysis of materials. This pan-European nanomaterials initiative will meet a changing world which will become known as the era of open innovation, with responsible partnering between all scientific and technological sectors. Equally, the rapid development of nanomaterials science and technology will advance our fundamental understanding of the nanoworld and the associated synthesis and characterisation techniques and will open up a whole new field of strategic research for the European research infrastructure, with the goal of developing new applications for the European industry.

The nanomaterials revolution

The end of the 20th Century saw significant advances in the design of 'nanomaterials', i.e. materials, components and products which may have a structure of only a few tens of atoms in size. Tailoring the properties of materials atom-by-atom offers the potential for improvement in device performance for applications across the entire range of human activity: from medicine to cosmetics and food, from informa-

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tion and communication to entertainment, from earth-bound transport to aerospace, from future energy concepts to environment and climate change, from security to cultural heritage. Nanomaterials will lead to a radically new approach to manufacturing materials and devices. Faster computers, advanced pharmaceuticals, controlled drug delivery, biocompatible materials, nerve and tissue repair, crack-proof surface coatings, better skin care and protection, more efficient catalysts, better and smaller sensors, even more efficient telecommunications, these are just some areas where nanomaterials will have a major impact.

This will affect so many sectors, and in many fields the pace of development will be so rapid, that failure to respond to the challenge with an efficient, timely, and co-ordinated European programme will threaten the future competitiveness of much of the European economy. Sophisticated materials and materials systems with novel properties and unheard-of performance will have to be conceived and designed in the decades to come, if our European high-tech industry is to remain competitive and if a high standard of living is to be assured for the European citizen of this 21st Century. It should be mentioned that at the industrial level, it is not economically competitive to build nanostructures atom by atom; therefore collective processing – where a large number of atoms are processed at the same time to build many nanoscale systems – must be developed.

The role of the European research infrastructure

Future knowledge-based nanomaterials research will critically depend upon materials characterisation methods, from common laboratory techniques to dedicated large-scale facilities. A fleet of sophisticated experimental methods will be needed to study all nano-aspects of new materials over a broad spectrum of length and timescales. No outstanding research on nanomaterials can be delivered without high performance characterisation tools and non-destructive methods.

Major assets in future nanomaterials research within Europe are the well-developed national and international synchrotron radiation, laser and neutron facilities. These facilities have been at the forefront of a wide range of scientific and technological developments over the last twenty years, supporting research in natural sciences (physics, chemistry, and biology), materials science and engineering, and in the development of advanced technologies and analytical techniques. This GENNESYS study has unravelled that these facilities will play in the nanomaterials revolution, and the insight that they can provide into the details of materials behaviour and mechanisms will be essential to realise the future potential of nanotechnologies for solving urgent problems of our society.

The analytical technologies provided by European research infrastructure offer a unique potential for the future development of nanomaterials: Highly brilliant and focused x-ray and neutron beams are able to interrogate all nanoscopic aspects of a given nanosystem ranging from structural, chemical, electronic, and magnetic to thermal properties. The tunability of all beam properties (energy, wavelength, focus, time structure, polarisation) allows one to explore a material with highest precision on a quantitative level. The penetrating power of high-energy x-rays and neutrons makes it possible to access deeply buried nanostructures and nanophenomena, and to study nanomaterials under industrially and environmentally relevant conditions in a non-destructive manner. The facilities offer dedicated support from sample environments via detector technology up to data analysis software.

The GENNESYS study has identified the urgent need for facilities which combine new instrumentation and beam lines with dedicated experimental support facilities, including modelling capabilities for the study of nanomaterials under real processing and operating conditions that are relevant to industrial research and development. GENNESYS has also disclosed those areas where dedicated upgrading of experimental methodology, instrument design, support structures and training of personnel must be addressed in order to render neutron and synchrotron radiation facilities most efficient to address future research needs for the development of nanomaterials and nanotechnology.

The range of applications for nanotechnologies

In order to structure the large field of nanomaterials and nanotechnologies, GENNESYS has subdivided the different areas of application of nanomaterials into research and technology fields For each of these fields, the key research challenges have been defined, the roles of synchrotron, x-ray and neutron methods identified, and a research roadmap for the next two decades outlined.

A. FUNDAMENTAL RESEARCH: GENERIC CHALLENGES

Fundamental research into nanomaterials behaviour is an essential prerequisite for generating the necessary scientific understanding of how nanostructures can be designed, synthesised and modelled. The complexity of this research demands advanced and high-performance analytical techniques to enhance the development and optimisation of the size, shape, structure and performance of nanomaterials.

1) Synthesis of nanomaterials and nanostructures

The challenges for nanomaterials synthesis lie in the design and tailoring of complex hybrid nanoparticles and "intelligent" or "smart" nanomaterials (nanotubes, functionalised surfaces, multi-layers, novel thin films and interfaces) with multiple functions for urgent applications.

The synthesis and assembly of new functional bio-nanomaterials, using nature's "tricks of the trade", will require an understanding of the complex relations between nanoscale structure and function in biological materials, and will enable advances in nanomedicine, bio- and biomimetic materials. This will lead to new applications in biosensors, implants, and tissue engineering, the development of which requires an understanding of the dynamic processes that are found in nature.

The tailored synthesis and processing of new particles and materials with multiple functions ("3rd generation nanomaterials") requires:

- Combinations of different synthesis techniques;
- In-situ characterisation under various environments and external fields, (e.g. gases, high pressure and temperature, biomedical applications, etc.);
- Continuous control of particle growth during all individual processing steps;
- Modelling the synthesis process:
  - i) to obtain enhanced understanding of the growth processes;
  - ii) to give guidance to the experimental work, in particular characterisation during synthesis;
  - iii) to develop a better understanding of advanced processing techniques to achieve optimised processing methodology for the fabrication of complex hybrid nanoparticles (incl. reproducibility and reliability);
  - iv) to tackle scale-up from the laboratory to industrial-scale synthesis.

The controlled design of novel nanomaterials requires a coordinated European effort. Synchrotron and neutron radiation facilities should offer their unique analytical potential to study in-situ the processes occurring during synthesis, and allow new developments for the creation of new nanomaterials. Future nanomaterials will be complex and multi-functional in nature, and the structures and properties required for particular functions will be derived by careful 'tuning' of their structure in the processing. To reach this goal, it will be important to be able to follow nanomaterials at all stages of their synthesis and processing.

A new European nanomaterials synthesis laboratory is proposed to keep Europe in a forerunner position for fundamental understanding of all synthesis processes which, for the "processing industry", will give Europe a competitive place in the global nanotechnology marketplace.

2) Nanomaterials phenomena and functions

Nanomaterials exploit physical phenomena and mechanisms that cannot be derived by simply scaling down the associated bulk structures and bulk phenomena. Surface phenomena will become more and more important compared to bulk phenomena. Furthermore, new quantum effects come into play which changes the way nanosystems work. It is the exploitation of these emerging nanoscale interactions which underpins all nanomaterials design. It is an essential challenge to understand the behaviour of given materials on all length scales, from the nanostructure up to the macroscopic response; and at timescales ranging from pico- and sub-picoseconds in molecular and electronic relaxation processes to micro- and nanoseconds in self-assembly processes, to days for long-term relaxation and degradation. The analytical access to this range of length and timescales, from the ultrashort to the ultralong, will be a future challenge for accelerator-based x-ray and neutron technologies in combination with complementary techniques.

Materials will be studied in the solid, liquid and gaseous phases, and at the interfaces between solids and liquids, and liquids and gases. Nanofluidics and nanomechanics play an important role for controlling the physico-chemical processes that are important for many advanced applications such as catalysis, energy conversion or storage using new nanotechnological approaches. It will be necessary to have beam lines at synchrotron radiation and neutron sources which can provide nanoscopic insight into the degradation processes of nanomaterials through in-situ experiments, with the necessary support equipment to perform experiments in 'real' sample environments, and simulate 'extreme' temperature, pressure, magnetic field, and corrosion.

3) Nanomaterials modelling

Modelling and computer-based materials design algorithms will become mandatory tools in testing our understanding of nanoscale processes and phenomena, which can be used in the development of tailored synthesis of nanomaterials, inhibition of degradation processes, and the planning of experimental programmes for nanomaterials development and assessment. For that reason, dedicated characterisation tools are needed, both to adjust model parameters and to check that the theory works or is correctly implemented in computer codes for simulation models.

There will be an increasing need to enhance our theoretical understanding of why particular phenomena arise in order to optimise synthetic processes, explain the mechanisms that lead to material degradation, and predict how nanomaterials properties can be improved. New ab initio models, where fundamental physical principles are used to predict the behaviour of materials at the nanoscale, will take advantage of the increased computing power available.

GENNESYS concludes that the creation of a European database of experimental data and modelling tools for nanomaterials and nanoscale physics is a strategic importance to underpin a sustainable development of key technologies. The database must be validated and data analysis methods must be standardised and easily accessible to all laboratories. The continuous development of this nanomaterials database und its use will be a vital tool for scientists and industrialists who will benefit from existing, ongoing and future research work in the nanomaterials domain.

GENNESYS study showed that a clever knowledge-based design concept must be implemented in which nanomaterials synthesis, the analysis of its atomistic structure, associated function and materials-specific modelling build a closed loop which leads to made-to-measure nanomaterials with highest efficiency. As this loop requires in particular the best analytic technology available, such a European nanomaterials synthesis centre should be built in close proximity and interaction with a large-scale facility for fine analysis of matter. Networks of the existing facilities should be quickly realised in order to be as efficient as possible and to avoid several laboratories to the same goals while other problems are not treated because of the lack of laboratories working on the subject.

B. NANOMATERIALS DESIGN

The GENNESYS study has reviewed a wide range of nanomaterials classes, and has highlighted the impact and novelty that their properties offer, and the potential they have in the production of new materials and designs. The study produced roadmaps for the whole spectrum of nanomaterials research, detailing the research avenues that should be pursued for the discovery and design of novel materials exploiting nanoscale phenomena. Synchrotron radiation, laser and neutron techniques must offer their unique capabilities for quantitative studies at a wide range of length and timescales for all the nanomaterials specified below.

In nanomaterials science, the development of new materials drives many fields of engineering; i.e. alloys with improved mechanical properties and reduced weight, e.g. to increase stiffness and at the same time save weight in aerospace or automotive industries. Composite materials follow the same trend, many of them mimicking the structure of biological tissues like wood, bone, shell, spider silk and many more examples. The use of such new nanomaterials will be essential to address major future global demands such as reducing energy consumption or the ecological impact of almost any product we use.

1) Structural nanomaterials based on metallic, ceramic and polymer systems will provide a step change in mechanical and thermal properties. They will be the basis for a wide range of innovations and new applications exploiting nanoscale effects. There are ambitious research goals in the production of nanostructures which are damage-resilient or even self-healing, materials that use nanostructuring to give dramatic improvements in strength, and the generation of new design concepts for industrial applications in diverse areas such as energy, transport and construction.

2) Functional or 'smart' materials drive forward developments in electronic, photonic, structural and magnetic devices. Nanomaterials will raise the development to a new level, employing novel physical, electrical and mechanical effects to make electronics which will be faster, lighter, cheaper, and easier to manufacture, and which will have low power consumption. Simple devices based on nanomaterials will deliver functions which would ordinarily require a more complex mechanism or component, such as the replacement of electrical connections by optical links and improved non-volatile computer memory. Designing materials operation in stringent environments (temperature, pressure, radiation etc.) is also needed.

3) Polymer nanomaterials will advance dramatically as the chemical and nanoscale structures of polymers are engineered to create new polymers with a multitude of structural and functional applications, ranging from polymers with improved biodegradability to new adhesives and novel electrical conductors. Biopolymers for the life sciences will use the principles of hierarchical assembly in living organisms and apply them to engineered materials and structures. The GENNESYS study concludes that revolutionary advances can be expected in this field.

4) Nanostructured coatings, composites and hybrids can be engineered to exploit a revolutionary combination of tailored properties, between coating and substrate, between composite matrix and reinforcement, and between the different components of a hybrid. The GENNESYS study has described how research into these classes of multi-component material systems will provide a new dimension of functionality, as they offer a route to produce combinations of properties that cannot be achieved by any other means. GENNESYS has compiled a roadmap for the development of these novel multi-phase material systems. To understand and tailor such processes will require dedicated analytical tools capable of probing and monitoring them at the nanoscale.

C. ENGINEERING PROPERTIES OF NANOMATERIALS

Nanomaterials research in the past has been directed towards the production of nanostructures as the primary goal, rather than to advance the formation of nanocomponents with defined properties and performance. There will be significant challenges in transferring the knowledge of new nanomaterials properties and mechanisms into the engineering design process, as we are not yet at the stage where nanomaterials can be designed and produced with known properties. Understanding is required of how nanomaterials can be joined without destroying their nanostructure and their function, how nanomaterials fail through corrosion, creep and fatigue, and how nanotribological mechanisms affect friction, adhesion, wear and lubrication. The overall lifecycle of the component must be assessed and understood, if accurate predictions are to be made. This could be demonstrated by monitoring in-situ the crack propagation along grain boundaries in steel alloys during corrosion using synchrotron radiation. This is extremely relevant to understand the mechanisms of material failure due to cracking of stainless steel under mechanical stress. In power plants, three-dimensional x-ray imaging could show: i) where the crack is situated relative to crystallites of different phases in the material; ii) how it propagates along the grain boundaries; and iii) how grain boundaries can be engineered to resist crack propagation. Modelling of materials from the nano-, to the sub-micron and macroscale is extremely important as well as the development of reliable multi-scale simulations for components reliability and lifetime predictions during in service conditions.

The GENNESYS taskforces have identified key research areas in which synchrotron, x-ray and neutron technologies will play a vital role to arrive at breakthroughs in tailoring the design, and in improving the performance in service of a broad spectrum of nanomaterials under real industrial operating conditions.

1) Nanojoining The GENNESYS study has highlighted potential techniques for nanojoining methodologies and technologies, and pinpointed research paths for successful development. Understanding the reliability and strength of nanoscale and nanostructured joints in-service is a great challenge. Existing knowledge and methods for large-scale welding and joining cannot be extrapolated to new methods and nanoscale effects. Synchrotron radiation- and neutron-based combinatorial techniques (imaging, tomography and diffraction) should be devised to measure stress in and around joints and welds, and to provide high-resolution imaging of joint performance and the development of damage during simulated operation.

In designing routes to combine nanostructured materials into larger assemblies, it is necessary to have joining techniques that do not disrupt the nanoscale structure. This is particularly critical as many joining techniques involve heat and/or mechanical deformation. Additionally, there is scope for developing materials which, by virtue of their nanostructure, allow for the creation of stronger joints than is the case with conventional materials.

2) Nanotribology The study of friction, wear and adhesion at the nanometre scale requires knowledge of surface interactions, chemical environment effects, lubrication, mechanical stresses, as well as biochemical concepts. This field is rapidly developing, but most of the applications that can be realised exploiting nanotribological ideas are still in an embryonic stage. Synchrotron, x-ray and neutron facilities are asked to devise appropriate analytical concepts which give new insights into the mechanics of local contacts at the nanoscale for the development of new wear-resistant nanocoatings and nanostructured lubricants, mechanisms of lubrication and wear at the nanoscale to minimise energy losses and damage in moving mechanical system, and mechanisms of local force generation at the nanoscale. Understanding of the latter will be critical in developing methods for molecular assembly by the movement and positioning of individual atoms and molecules. Understanding dissipative mechanisms at the nanoscale is an important challenge for developing useful nanosystems.

3) Life cycle of nanomaterials The lifetime of an operating nanoarchitecture is limited by fracture, fatigue, creep, corrosion that will differ significantly from those that operate in ‘conventional’ structural materials. A mechanistic understanding of the damage mechanisms operating at the nanoscale, obtained using in-situ synchrotron radiation and neutron experimentation, will be critical to generate the knowledge base needed for the reliable application of nanomaterials in engineering applications. The understanding of nanodamage mechanisms is needed as input in simulation models.

D. CHALLENGES IN NANOMATERIALS TECHNOLOGIES

The enormous potential impact of nanomaterials for new technologies has been highlighted by the GENNESYS study. The opportunities for nanomaterials research and development have been defined for a broad spectrum of technological application areas to deliver unprecedented impact in fields encompassing faster information exchange and new multi-functional computer systems enhanced healthcare, with new drugs through bio-nanotechnologies and nanotherapies in medicine; more energy-efficient transport encompassing light-weight structural materials; reduced pollution and carbon emissions; and technologies for safety and risk reduction. The goal is the enhancement of these technologies for improved quality of life, through the development and production of new materials with novel properties. These breakthroughs critically rely upon advancing our fundamental knowledge of nanomaterials. It is the future strategic role of the European research infrastructure to provide this information in due time and develop a responsible partnering with industry for realising the new paradigm of open innovation.

In the decades to come, a series of difficult problems will have to be addressed, from global warming and energy consumption to affordable medical care. In many cases, nanoscience and technology will contribute considerably.

1) Information Technology

The tremendous progress of micro- and optoelectronics in the past decades is driven by the fabrication of ever smaller structures, increasing the number of elements per area and decreasing the cost per element exponentially. Currently, the dimension is in the range, and conventional production will meet its limits in a few years. New concepts such as the use of strained silicon to increase performance have to be pursued further; eventually new materials and completely new device concepts will have to be introduced. Self-organised nanostructures like quantum dots and quantum wires should improve significantly the performance of optical devices such as semiconductor lasers. As we decrease the dimensions of systems, similarly to the sound barrier, we shall soon meet a quantum barrier where basic properties change owing to the appearance of new quantum effects arising from the small size of the system.

The future prosperity of the information technology industry strongly depends on further successful down-scaling processes, creating new devices with higher functionalities, greater flexibility and reliability, and improved performance. Nanoscience and -technology will provide important basic approaches for improved functionalities and new device concepts. The new nanoelectronics will give a step change in functionality – higher speeds, reduced power consumption, reduced complexity – that will provide novel computer, photonics and informatics applications over the next 20 years.

In microelectronics and photonics, new developments such as quantum communication and computing, data storage using new materials, and concepts such as magnetic semiconductors and spintronics, will revolutionise capabilities. Most of these concepts are based on nanostructures, and in most of these cases structural studies using synchrotron and neutron sources are essential.

2) Health: biological and medical applications

The entire scope where nanomaterials impact human health, through medicine, dentistry, cosmetics, food and agriculture, has been evaluated. The healthcare industry is dependent on drugs and drug delivery systems for disease control and improving the quality of life. New drug systems with controlled release can be developed using nanoengineering, and the delivery of drugs into the human body is much simplified by exploiting nanoscale effects i.e. delivering just the amount of drugs necessary to patients allows decreasing the amount of drugs and the impact of pollution since the excess is often released in the environment.New ointments which exploit nanoscale binders will have offshoots into the cosmetics industry, which will be able to exploit the research and development needed for the full exploitation of nanomaterials in healthcare.

Nutrition is critically important for health and the quality of life. Increasing demands for more efficient food production and processing, the possibility of engineering foodstuffs for improved nutrition, and the development of foodstuffs designed to be suitable for people with allergies or nutritional disorders will all require a step change in our ability to manipulate the structure of materials at the nanoscale. In particular, being able to formulate foods which can be successfully processed is of fundamental importance. Prototype production facilities will need to be developed which can be operated at x-ray and neutron facilities for real-time and in-situ studies of the development of relevant structure and the associated mechanisms.

3) Manufacturing engineering

Nanomaterials have to meet the demands facing new structural materials, reduced energy consumption, and reduced life-cycle costs. Advances include reduced fuel consumption and operating costs, reduced or zero emissions, improved capacity and comfort and reduced noise. Breakthroughs in nanomaterials engineering depend on how precise we can "see" the relevant structures and how they change during a process. This puts serious demands on tailored analytical tools ranging from diffraction, imaging, microscopy, tomography and spectroscopy with highest spatial resolution (<50 nm).

Many 'traditional' materials embody the principles of nanomaterials engineering in developing their structure at the nanoscale. There are still significant advances to be made in many fields of metallurgy. Synchrotron, x-ray and neutron methods have been instrumental in many major advances in our understanding of the fundamental mechanisms of materials mechanisms and performance; these instruments and methods will continue to help identifying new mechanisms in nanomaterials, using much higher spatial resolution.

4) Nanomaterials in energy technologies

Climate change and the security of energy supply are two of the most pressing concerns facing both developed and developing countries alike. To tackle energy consumption and associated problems, no other way than using renewable sources and developing nuclear energy will be possible in the medium to long term. Saving energy and an efficient use of it are the basic requirements in this evolution.

The potential impact that nanomaterials can make in this area is truly enormous. If current projections are correct, they could achieve transformational changes in the way we convert and use energy, providing a sustainable, clean, efficient and above all decarbonised energy system.

The study of materials for energy is extremely broad and covers a very diverse set of materials embracing functional, chemical and electronic energy materials. Development of nanomaterials for these applications will require, for all the different materials types, the probing of structure at all length and time scales.

There are many cases where the application of nanomaterials will be central to these transformational changes. Nanomaterials for Li-battery technologies are in development, and nano-$LiFePO_4$ as a cathode is a good start but further developments in nanomaterials are necessary to engineer the high power batteries needed for hybrid electric vehicles.

Improved solar cell concepts are based on semiconductor nanowires (the "high-tech solution") or new organic compounds (the "low-tech solution"). For improved batteries such as Li-ion-cells, covering the electrodes with nanostructures might solve the problem of expansion/contraction during the charging/uncharging cycle, which is at the moment a big issue in battery lifetime and safety. Solar cells will be important in the future but the date at which this will be implemented on a large scale depends much on the cost of photovoltaic cells which are for the moment too expensive. Progress in mastering thin inorganic and organic films is urgently needed.

Nanomaterials are seen as one of the most promising routes to achieving targets for solid state hydrogen storage, and new nanostructures are emerging that offer fast ion transport along interfaces that could revolutionise electrochemical devices such as fuel cells. The application of nanomaterials in photovoltaic devices are as numerous and as important, ranging from nanomaterials for dye-sensitised cells to light concentrators and absorbers.

The importance of all these devices to our society and its future cannot be overstated and whilst conventional materials have an important role to play, only by fundamental studies of nanomaterials the key breakthroughs in energy technologies will be achieved.

All mentioned developments rely heavily on advanced material characterisation; synchrotron radiation and neutron scattering play an important role here, and are especially powerful for the investigation of nanostructures incorporated in a device, eventually even during device operation e.g. change of Si-nanowires in a Li-ion battery during charging/discharging. Neutron and synchrotron x-ray will be the core facilities used to achieve the insights needed for the breakthroughs in these new energy technologies.

5) Environment

In natural and man-made environment, nanotechnology will help to solve problems like soil and groundwater remediation, air purification, pollution detection and sensing. The same is true for man-made waste reduction including nuclear waste which also requires developing safe geological disposal with methods acceptable for society. A better prediction of climate change is directly linked to the understanding of the role of aerosols (nanoparticles) in the atmosphere.

6) Security and safety

Nanotechnology will bring new answers to the prevention and protection against terrorism threats, or against natural and industrial accidental risks. Nanotechnology will also provide efficient response to the security and safety of critical installations and the environment.

7) Culture and art

Nanoscale and microscale studies of archaeological artifacts or historical objects will help to understand their history, past technological and artistic skills as well as past climate and environment. Nanotechnology will also help in finding new protection of precious objects which are part of cultural heritage and a huge source of revenue from tourism.

E. NANOMETROLOGY RESEARCH AND STANDARDISATION

A new generation of nanomaterials will require a new concept of measurement techniques for the characterisation and the determination of their physical properties. These nanostandardisation methods will also become increasingly important in proving validation of novel measurement techniques in order to assure their reproducibility, quality, robustness and accuracy. Alongside the development of any new measurement technique, it is vital that it is applied in a standard, reproducible way. Modern industry relies heavily on standardisation of measurement, processes, methods and products, and on the use of Standard Reference Materials. GENNESYS strongly recommends exploring the unique analytical portfolio offered by the European research infrastructure to produce new nanostandards.

Good practice in metrology requires standardisation of any new or improved measurement techniques, standardisation in information and data reporting and interpretation, and globally-accepted standards for measurement. All of these are critically important for the study of properties and structures at the nanoscale.

It will therefore be important for new instruments developed at synchrotron radiation and neutron sources to carefully reflect on the requirements of industrial users in having standardised sample environments and software for experimental planning, execution and analysis.

Reference nanomaterial standards will be mandatory to ensure the quality of the scientific deliverables, as they will provide benchmarking of the data generated.

The establishment of a European meeting point for nanomaterials metrology is essential for the exploitation of this emerging discipline, and to help ensure its successful growth and the promotion of the GENNESYS platform.

F. IMPACT, INFLUENCE AND BENEFITS FOR SOCIETY

Nanomaterials may generate products which improve the quality of life for individuals. Thus, it is important to prepare for a European industry which can compete openly in the international market with its products and processes.

Nanomaterials will bring benefits throughout society and its activities:

- In economy, science and technology are the principal drivers of economic growth and quality of life. Research, particularly nanomaterials research, has widespread impact in health, information, energy, and many other fields where there is major economic benefit to the commercialisation of new technologies.
- Concerning energy efficiency, nanomaterials research will have a great impact, as new nanomaterials will allow higher temperatures and hence a more efficient operation of power plants, and enable the development of new energy production systems based on nuclear, solar, and renewable sources.
- In medicine and health care, nanomaterials will provide new drugs and new therapies, and cures for currently chronic and fatal illnesses. Important areas of research will be the application of nanomaterials in tissue engineering and medical imaging. The potential application of nanotechnologies has immense capability and promise for advanced diagnostics, improved public health and new therapeutic treatments.

Nanomaterials technology will reach large-scale production if one or more of the three following conditions are fulfilled:

- Nanomaterials give the same performance as conventional materials at a reduced cost;
- Nanomaterials give a better performance at the same cost or a price marginally higher;

Apart from the unquestionable benefits, the risks associated with nanoscale materials have also to be addressed. History has shown that new science and technology often cause fear and misunderstanding in society. This holds also and in particular for the field of nanomaterials, because their developments also constitute 'unknown' and invisible aspects. Nanomaterials processing techniques can be dangerous for health and studies on animals have demonstrated this. Great research efforts should be made to investigate health impacts and methods to prevent them.

Synchrotron radiation and neutrons may help in defining the boundary conditions for risks and to build up a robust database for a mechanistic understanding of nanomaterials behaviour. The use of advanced, established experimental techniques may help to alleviate some of the perceived problems with employing nanomaterials in consumer products.

Systematic fundamental research is needed for understanding toxicity and the impact of nanomaterials in the human environment. Research is also required into how and why public perceptions of nanomaterials and nanotechnologies are formulated, and what steps are required to reassure the public. Public education of the scientific facts about nanomaterials, and the benefits to health, the environment and to economic prosperity, need to be communicated clearly.

A close collaboration between scientists, industrialists and government is needed to safeguard this new nanomaterials research field. To stay competitive on a global market, to secure energy supply, and to meet the environmental challenges of our industrial society are the main socio-economic driving forces for the future development of the European economy. The potential impact and benefits of nanomaterials simply cannot be ignored.

G. IMPLICATIONS OF GENNESYS FOR EDUCATION AND TRAINING

The GENNESYS conclusions on the need for a pan-European strategic action plan for the development of tailored nanomaterials and nanoarchitectures, in order to specifically contribute to solve or mitigate an urgent technological problem requires breakthroughs in nanomaterials research by an interdisciplinary and cross-sectorial effort. This in turn requires that the materials scientists and engineers involved in this endeavour are experts in their field and have the necessary literacy in neighbouring fields as well as in industrial practice. Furthermore, they should be able to move freely within Europe and understand managerial, economical and societal issues.

During their work, the GENNESYS task forces understood from industry that this type of scientist is rarely available today. GENNESYS has thus devised a new education scheme and training structure and has made a distinct proposal of how to establish a European education in nanomaterials science which involves all sectors engaged in the GENNESYS initiative (see below).

For Europe to continue to compete alongside prestigious international institutions and programmes on nanomaterials, it is important to create a "Europe Elite College".

1) European Nanomaterials College

This type of nanomaterials scientist and engineer with the expertise and skills mix described above is currently not produced in any of the universities in Europe. GENNESYS has devised a syllabus for a European Master's and PhD course which assures a research-focused education, a close involvement of industry and national and European research labs, as well as the necessary literacy to work efficiently in a multi-disciplinary research and engineering consortium. This new syllabus is the mission of a new European Nanomaterials College. This should be a new institution, involving 'satellites' of leading Universities and other institutions throughout Europe. The partner of this new college should be the GENNESYS institutions, i.e. the European universities, national and European research labs, industry and the European research infrastructure.

2) International collaboration

The GENNESYS foresight and strategy document addresses urgent problems which have a global dimension, such as new concepts for future energy and environment. Thus, it is very strongly recommended to establish international collaborations with United States and Asia as well as other industrial countries.

3) Industry partnerships

Nanomaterials and technologies have great potential for the future, and a correspondingly strong demand for advanced analytical techniques. This has long been realised by the pharmaceutical, cosmetics and information-technology industries, with future applications in the energy, aerospace, chemical engineering and automotive sectors.

In a future new era of open innovation, partnerships across disciplines and among universities, government laboratories and industry are essential to leverage resources and strengthen interdisciplinary research and connections to technology. A responsible partnering between academia and industry will enable cross-disciplinary research and provide awareness of technological drivers and potential applications.

The European Commission should provide incentives for formation of sustainable strategic partnerships between universities, industrial labs and research centres, and the European research infrastructure for the advancement nanomaterials science and technology. Raising the profile and intensity of interdisciplinary research in nanomaterials will help to restore the leadership and activity in European research that generated many of the advances in the 21st century that benefit our lives today.

These research and development partnerships should be encouraged in order to:

- Enable cross-disciplinary and cross-sectorial research in key fields;
- Create a new spirit of open innovation;
- Improve academic knowledge on industry priorities and needs;
- Improve industrial knowledge on nanoscience discoveries;
- Exploit the existing European research infrastructure for nanomaterials development
- Assemble teams that can recreate the fertile research environment of the large industrial research labs;
- Develop the commercial exploitation and patenting of new technologies.

These partnerships should be fostered by:

- European and national funding;
- Encouraging university and research labs internships and sabbaticals in industry.

For a future strategic collaboration between industry and the European research infrastructure, it is prerequisite to overcome the following three key barriers:

- Lack of expertise and lack of understanding of complex analytical tools;
- Concerns over commercial confidentiality and intellectual property;
- Non-existent standardised analytical setups.

In turn, there are challenges for the large-scale facilities:

- Standardisation of analytical concepts and set-ups;
- Certification of measurement procedures;
- Faster access to the European Research infrastructure for academics and industrialists;
- Support for non-specialist users of the facilities before, during and after the experiment;
- Close cooperation between instrument scientists and users;
- Predefined sets of standard sample environments.

H. IMPLEMENTING GENNESYS: CHALLENGES AND REQUIREMENTS

The development of nanomaterials and nanotechnology in Europe faces several challenges:

- Nanomaterials science in Europe is severely fragmented into different disciplines, sectors and member states;
- Its critical role not appreciated by the public, because it takes place in the background;
- The European nanomaterials community and the European research infrastructure are largely unaware of each other;
- There is no efficient platform for continuous knowledge transfer between academia and industry.

With the implementation of the GENNESYS vision, all these problems could be overcome or at least substantially mitigated. It is hoped that the roadmaps presented in this GENNESYS European Nanomaterials Strategy Study will provide a point of reference for policy-makers, lab directors, university rectors and industry management. It is envisaged that GENNESYS will serve as world-wide platform for scientists to foster future collaborative, cross-disciplinary research and development, and to stimulate growth in the commercial exploitation of nanomaterials science and technology in Europe.

I. GENNESYS SCIENCE CENTRES

To be able to take the world lead in nanomaterials – discovery, scientific understanding and industrial innovation – Europe must concentrate its best researchers, research facilities, research equipment, research expertise and research infrastructures to tackle the key challenges in nanomaterials research. While similar efforts have already been made in the US, the GENNESYS recommendation goes a step further.

Successful nanomaterials research for solving a given urgent problem of our society will require a multi-disciplinary approach across all sectors, incorporating expertise in physics, chemistry, biology and engineering as well as computational and theoretical tools; and a broad spectrum of advanced and dedicated analytical methods which interrogate the nanomaterials and nano-architectures in-situ, non-destructively, at all relevant length scales and under a range of environmental and operating conditions. GENNESYS taskforces strongly recommend that synchrotron radiation, laser and neutron facilities must play a strategic role in this research effort.

GENNESYS recommends creating European Centres of Excellence in nanomaterials research with a clear mission to solve an urgent problem. In order to capitalise on the existing unique analytical potential of the European research infrastructure, those Centres should be built at large-scale facilities for the fine analysis of matter. Science Centres will focus onto fundamental research in nanomaterials science under guidance of an academic research lab consortium and provide the molecular database for robust technology development, Technology Centres will focus onto the development of working "nanosolutions" in all key technologies under the guidance of industry and other partners.

These centres will provide a strategic, knowledge-based pathway from fundamental science to applications with the possibility of the creation of new spin-off companies. These centres offer important spin-offs for students to understand computational methods and to engage with a wide range of experimental methods and applications, providing a basis for them to become successful researchers and industrial innovators. Such centres will also attract, train and develop the next generation of leading young scientists who are vitally-important for a growing, modern economy.

Conclusions and recommendations

Nanomaterials science and technology will provide breakthroughs for many technologies in the future, and solutions for urgent problem in our society. In order to leverage the fragmented knowledge in Europe for a strategic pan-European nanomaterials programme, a joint effort of all sectors of research and innovation is necessary, including the existing highly developed European research infrastructure.

A close collaboration between scientists, industrialists and the government is needed to safeguard this new nanomaterials research field. To stay competitive in a global market, to secure energy supply, and to meet the environmental challenges of our industrial society are the main socio-economic driving forces for the future development of the European economy, and the potential impact and benefits of nanomaterials simply cannot be ignored.

GENNESYS is a foresight and strategy document compiled by using expert input from the education, science, technology, policy-maker and governmental authorities. It has demonstrated that a stepwise improvement in Europe is needed in order to take a leading position in the world of nanomaterials science, technology and industrial exploitation. A strategy must be developed and delivered to ensure future impact on economy and society, and success in this grand challenging new world.

The conclusions of GENNESYS can be summarised as follows:

- The study gives an overall picture of the future research needs in the large spectrum of nanomaterials and highlights the important roles of advanced analytical equipment in reaching breakthroughs, especially the synchrotron radiation and neutrons facilities. The study is a reference work for scientists, research managers, industrialists and policy-makers to design new programmes and guide future research in nanomaterials.

- GENNESYS indicates the potentials for industrial innovations of nanomaterials; it gives directions for new targeted processing techniques. Synchrotron radiation and neutrons are ideal tools to measure progresses in-situ.

- Nanomaterials research is thinly spread over many European countries and institutes. GENNESYS provides a mechanism to bring the efforts together in setting up GENNESYS Science and Technology Centres throughout European at large-scale facilities. This is a necessity to keep Europe a forerunner in this field.

- The European GENNESYS Centres of Excellence bring the European talent together – scientifically, industrially, socially and economically. They are multi-disciplinary centres where nanoscientists from all European countries are welcome. They offer opportunities to research institutes and universities of central- and Eastern Europe to participate actively. The centres should have the theme of "Science" or "Technology" orientation. They could be compared to the CERN organisation in high energy physics in Geneva.

- GENNESYS highlights the importance of creating a European/international institution for nanomaterials where talented students could prepare for a brilliant career. This institution, with satellites around various large-scale facilities, recognised universities and industries, will become competitive with the best US and Japanese school in nanomaterials. The institute should also deliver qualifications that are recognised throughout Europe.

- The GENNESYS study analyses a wide spectrum of nanotechnologies. It hints towards solutions in the complex energy question, particularly related to new energy sources or to the improvement of existing sources. It also studied completely new topics such as nanomaterials for security and safety, nanopharmaceuticals and nanofoods, the role of "nano's" in global climate change, etc.

- The study pinpoints the advantages of nanomaterials but analyses in depth the research needs to combat the toxicology and nanoprotection problems and tries to delaminate the borders/boundaries between danger and no risks. Synchrotron radiation and neutrons are of great importance in studying the mechanisms of dangerous nanospecies in the body.

- In order to cope with the challenges and needs of nanoscience and technology, considerable improvements are needed also with large-scale facilities such as synchrotrons and neutron sources.

This has technical aspects as well as organisation aspects (availability, ease of access) and educational ones: e.g. extreme focusing nanobeam stations, small neutron beams, transferring scientific results from laboratory conditions to realistic industrial ones, etc.

- To achieve efficient work and collaborations between large-scale analytical facilities and nanoscience and technology, the creation of GENNESYS type analytical centres is essential.

Europe will need to invest in the next generation of synchrotron radiation, laser and neutron facilities, offering higher fluxes and more brilliant probes, and providing significant and necessary advances with regard to resolution, sensitivity, and data acquisition. A continuous investment is needed in the upgrading of Europe's synchrotron x-ray sources, with improvements in equipment and instrumentation, new ancillary equipment to support new experimental methodologies, and a rolling programme of upgrades to ensure that Europe's synchrotron sources remain at the forefront of research in nanomaterials science and technology.

- It is suggested that the European Commission, in collaboration with the European Science Foundation and other European authorities and national funding agencies, should establish a European body with the mandate to coordinate all nanomaterials activities and large-scale facilities in Europe.

- GENNESYS recommends creating a European College for Nanomaterials Science, Science Centres and Technology Centres of Excellence for research, development and exploitation of nanomaterials in closest interaction with the European research infrastructure. The European synchrotron radiation, laser and neutron facilities have the most advanced analytical equipment and a solid and proven infrastructure of scientists and equipment.

Governments should promote the creation of new European Centres of Excellence and an International Institute for Nanomaterials Education, to be coordinated by the European Commission and/or relevant agencies.

Helmut Dosch
Marcel H. Van de Voorde

Max-Planck-Institut für Metallforschung

PREFACE

The European GENNESYS Project on Nanomaterials Science and Technology

During the last decade, worldwide attention has been drawn to the enormous potential of nanoscience and nanotechnology. Today, novel nanomaterials are no longer the concern of scientists alone; rather, they are starting to have a real effect on many industrial technologies, including electronics, telecommunications, chemicals, transport, medicine, energy, and the environment. These technologies all depend on the development of materials that can withstand the highest mechanical and thermal loads, transfer data at the greatest speeds, safely store data in the smallest dimensions, ensure biocompatible transplants, remove monoxides from car exhausts, or separate protons and electrons infuel cells. There are great expectations for the future of nanomaterials science, and most countries have already established nanomaterials science and technology programmes.

As material systems and device structures become nanosized and nanostructured, new challenges are emerging: how to grow and design these artificial material structures in a precise and reproducible manner and secondly, how to analyse their three-dimensional structure, properties, and functions with the highest level of precision. It is apparent that detailed knowledge of the chemical, electronic, and magnetic structure of nanomaterials is a prerequisite to being able to tailor their functions in a controlled way.

Modern analytical technologies based on synchrotron radiation and neutron facilities carry the potential to investigate the chemical, electronic, and magnetic structure of any given material structure under any possible environment in a non-destructive way. In the last 30 years, x-ray and neutron technologies have experienced breathtaking development in new types of sources, sophisticated analytical schemes, and robust theories. We have witnessed a revolution in x-ray techniques with the availability of synchrotron radiation. Modern synchrotron radiation facilities provide highly brilliant x-ray light with tailored properties. Synchrotron radiation and neutron facilities have developed revolutionary new ideas and experimental schemes to characterise nanomaterials, nanophenomena, and nanoprocesses. These schemes encompass diffraction, diffuse scattering, inelastic scattering, magnetic scattering, tomography, spectroscopy, microscopy, and all kinds of highly sophisticated combinations. The future development of x-ray nanobeams with beam size down to a few nanometres will lead to a further revolution in x-ray technology. Future pulsed neutron sources will enable new kinds of investigations into the structure and dynamics of magnetic, soft, and biological materials.

While twenty years ago, it was something very special to carry out an experiment at a synchrotron radiation or neutron facility, research at dedicated synchrotron radiation and neutron facilities has become routine today. These facilities produce tailored radiation and deliver it with a reliability of close to 100%, together with an impressive arsenal of sophisticated instrumentation and dedicated sample environments. They also have learned how to optimise user access and operation. Users are now assisted by a "local contact team" who assist them in getting the most information from their samples. Facilities also have specialised theory groups that offer professional help in quantitative data interpretation. In a nutshell, current synchrotron radiation and neutron facilities house a mature analytical potential of the highest calibre. This potential will prove essential in overcoming analytical challenges in the development of advanced materials.

Many materials scientists have only a passing knowledge of the analytical potential provided by synchrotron radiation and neutron facilities and their use in their own research. Likewise, the operators of these facilities do not know the roadmaps of nanomaterials development and what the current and future analytical needs in the development of novel materials really are.

In autumn 2002, a high level group composed of nanoscientists and experts from the synchrotron radiation and neutron facilities met in Grenoble to discuss the future role of the synchrotron radiation and neutron facilities for the development of nanomaterials and nanotechnology in Europe. There it was decided to launch a new European initiative named GENNESYS (Grand European Initiative on Nanoscience and Nanotechnology using Neutron and Synchrotron Radiation Sources), in order to bring these rapidly developing communities together. At a European kick-off meeting in November 2004 in Stuttgart, the overall strategy for the GENNESYS enterprise was formulated and approved.

A primary mandate of the GENNESYS initiative has been the collection of the relevant information from European and worldwide research laboratories about the future trends and needs in advanced analysis for the development of nanomaterials and nanotechnology. Recognised scientists and technologists familiar with these topics have been asked to contribute to this exercise. The entire European research community (universities, research institutes, funding agencies, and private company laboratories, as well as policymakers representing individual countries, and the European Community), is actively integrated into this unique European project.

A further task of the GENNESYS initiative has been:

- To assess the state of the art of nanomaterials science and technology;
- To highlight and prioritise future challenges and research needs, and set out a suitable time frame for addressing them;
- To pinpoint the areas of research in nanoscience and nanotechnology that will most benefit from joint research strategies with synchrotron radiation and neutron sources;
- To review and forecast the effects which increased use by nanomaterials scientists will have on large-scale facilities;
- To formulate a European research programme for "nanomaterials science and technology exploiting the analytical potential of existing and emerging European synchrotron radiation and neutron facilities."

The final results have culminated in the compilation of this GENNESYS White Paper, providing a vision of progress in this field and any new kinds of joint research strategies, research partnerships, new experimental equipment, novel operating modes of synchrotron radiation and neutron beamlines that will have to be developed. Special efforts will ensure that sufficient resources will be made available to promote this important research initiative.

The GENNESYS White Paper has produced new insight into the problems of nanomaterials development and has arrived at conclusions and recommendations about what must be done to advance this important field in Europe. The GENNESYS task forces revealed an urgent need for in-situ and non-destructive analysis of nanophenomena and nanomaterials and a strong need to monitor not only the function of a material but also its performance and its failure behaviour on the atomic scale. They have also brought to light that the synthesis of nanomaterials needs improved in-situ monitoring of the relevant growth parameters. The structure of functional interfaces and its change during operation will become of key importance for future nanotechnologies; thus, the in-situ investigation of such buried interfaces under environmentally and technologically relevant conditions must become a major effort. GENNESYS also disclosed a considerable need for the characterisation of materials on all length scales, high-throughput analysis of materials, combinatorial capabilities and robotic analysis. A most promising future field of in-situ analysis is real-time x-ray and neutron study of microscopic and mesoscopic processes. The development of catalysis, for example, requires demanding real-time x-ray studies beyond the picosecond time resolution, a request that has been put forth by industry. Likewise, the use of synchrotron radiation and neutron facilities for nanometrology and nanostandardisation will rapidly emerge and grow.

For key areas in the development of nanomaterials and nanotechnology, GENNESYS recommends multidisciplinary Science Centres and Technology Centres to be installed at synchrotron radiation and neutron facilities. This new type of institute will focus all necessary research efforts, attract the best scientists in the field, and provide the essential (synthesis, analysis, modelling) infrastructure, including tailored analytical technology from the associated synchrotron radiation or neutron facilities, for direct characterisation and monitoring of phenomena and processes.

The GENNESYS project also points to several critical problems in Europe's nanomaterials research which have to be overcome in the near future. Among these problems are the fragmentation of efforts in nanomaterials research, the lack of clear European research careers in nanomaterials science as well as the lack of public awareness of the importance of fundamental research in nanomaterials science for the advancement of our society and for the benefit of the European citizen.

In addition, the GENNESYS project has arrived at recommendations for materials science curricula. Since nanomaterials science is an interdisciplinary research effort merging the traditional fields of physics, chemistry, engineering, and biology, the appropriate education of young scientists is essential. One dangerous option currently being pursued in Europe is to replace the traditional research fields by a general materials science curriculum. The development of advanced materials, however, requires experts in a particular field who do not 'swim along the coast'. Finding the proper education scheme which produces top-notch experts who at the same time, have the necessary literacy in neighbouring fields, is an unsolved challenge.

The GENNESYS team members are convinced that the initiative will substantially contribute to the solution of all these rather difficult problems. Europe is a melting pot of different nations and cultures. This multicultural character carries a unique potential that must be exploited much more efficiently in advancing science and technology. Materials science, the textbook example of 'border-crossing' or intersecting research fields, could serve as a model to demonstrate what joint European forces can achieve. This is part of the broader vision of GENNESYS.

I am deeply indebted to all my colleagues who have devoted considerable efforts during the last years in making this GENNESYS White Paper possible. I am convinced this document will have a profound and sustainable impact on the development of nanotechnology in Europe.

Helmut DOSCH

Chair of the GENNESYS Initiative
Director Max-Planck Institut für Metallforschung, Stuttgart (DE)

FOREWORDS

Die großen Herausforderungen unserer Zeit – Klimaschutz, zukunftsfähige Energieversorgung, Bekämpfung von Krankheiten – werden wir nur bewältigen, wenn wir unsere Kräfte in der Forschung noch stärker bündeln und gemeinsam nach Lösungen suchen. Insbesondere Nanomaterialien können bei der Gestaltung unserer Zukunft eine wichtige Rolle spielen. Sie liefern Bausteine für neue Technologien und ermöglichen damit nachhaltige Energiekonzepte und Transportsysteme, eine effizientere medizinische Versorgung und neue Informationstechnologien. Eine europäische Strategie für Nanowissenschaften und Nanotechnologien, die alle relevanten wissenschaftlichen Disziplinen berücksichtigt und neben Universitäten und außeruniversitären Forschungseinrichtungen auch Partner aus der Industrie einbezieht, wäre ein wichtiger Schritt auf dem Weg zur Entwicklung solcher maßgeschneiderter Nanomaterialien.

Die GENNESYS-Studie ist ein Meilenstein in den Nanowissenschaften und Nanotechnologien. Unter der Leitung des Max-Planck-Instituts für Metallforschung in Stuttgart haben Wissenschaftler mit unterschiedlichem Hintergrund und Wirtschaftsvertreter verschiedener Branchen gemeinsam mit den Betreibern der europäischen Forschungsinfrastrukturen dieses – für die nächsten Jahrzehnte wegweisende – Referenz-Dokument zusammengestellt. 800 weltweit führende Materialwissenschaftler und Ingenieure identifizieren in ihren Beiträgen Forschungstrends und -bedarfe. Und sie benennen die Herausforderungen, die wir meistern müssen, damit Europa seine globale Spitzenposition in den Nanowissenschaften und Nanotechnologien behaupten und weiter ausbauen kann.

GENNESYS zeigt, dass Schlüsseltechnologien bahnbrechende Innovationen hervorbringen können. Eine entscheidende Rolle spielt dabei die europäische Forschungsinfrastruktur mit ihren Neutronen- und Beschleuniger-basierten Röntgenquellen. Ihr einzigartiges analytisches Potenzial ermöglicht eine neue Strategie für nachhaltiges Wachstum in Europa.

Ich danke der Max-Planck-Gesellschaft, die dieses ambitionierte Projekt ermöglicht hat, und allen, die an dieser Studie mitgearbeitet haben.

Annette SCHAVAN

Bundesministerin für Bildung und Forschung
Federal Minister for Education and Research, Berlin (DE)

Nanotechnologies and nanoscience is a rapidly emerging field of research with enormous potential for societal and economic benefits. Time and time again, scientific discoveries have resulted in innovations in the fields of medicine, chemistry and energy, to mention just a few, that have a profound impact on our daily lives.

Although the pace of development is very fast, fundamental science still plays a significant role due to the unique challenges of manipulating and characterising matter at the nanoscale.

World-class research infrastructures often play a key role in unlocking the mysteries of fundamental science. However, research infrastructures are expensive. In current times of global economic downturn, it is more important than ever to overcome the fragmented infrastructure spending across the EU and even to increase the overall investments. Within the European Research Area (ERA) we have the ambition to maximise the effectiveness of resources available.

The European Strategy Forum on Research Infrastructures (ESFRI) has compiled a roadmap for pan-European research infrastructures. In December 2008, there were 44 proposals being developed for new large-scale or European distributed research infrastructures and no fewer than seven of these directly address materials sciences. This highlights the importance of the field of science that the GENNESYS report represents.

To achieve high added-value in an emerging knowledge economy, outstanding knowledge is fundamental. In this respect, Europe needs bright scientists, supported by efficient research infrastructures, to deliver on the promise of nanotechnology. I therefore welcome the GENNESYS study which has been drafted in the spirit of ERA and which will certainly become a landmark document in its field.

Janez POTOČNIK
European Commissioner for Research, Brussels (B)

European academic institutions are rich in tradition and have contributed significantly to the present state of advanced technologies and the competitiveness of European industries. However, these institutions often have difficulties competing for technological leadership against rivals in the USA and Asia. We therefore should aim at further enhancing the creativity and efficiency of the output of research and the investigative talent of young scientists at these institutions. This can be achieved by promoting coordinated collaborations between European universities and research centres, particularly in fields expected to create new opportunities for European industry.

Nanomaterials science is one such field. The compiling of this GENNESYS study is a welcome step in bringing the nanomaterials scientist's message to a wider audience. It shows the important role of nanomaterials science in modern technological development and the necessity of top-class university training necessary for innovative products of tomorrow. It will help to raise the profile of nanomaterials science as a discipline.

Europe needs students with training in multi-disciplinary themes: materials, physics, chemistry, biology, mathematics, informatics, and engineering and they require extensive experience with capital-intensive, large-scale research instrumentation specifically in the fields of synchrotron radiation and neutron sources. Highly trained and talented students, scientists and researchers are needed at all levels of nanomaterials, from industry to academia. We have to make this field attractive in Europe. Obstacles hindering students and researchers coming here from outside Europe should be removed and the European research infrastructures in this field should be highly competitive.

GENNESYS proposes a model approach to the challenges in the field of nanomaterials and that is why I give my wholehearted encouragement to this initiative.

Pascal COUCHEPIN

Former President of the Swiss Federal Council
Head of the Federal Department of Home Affairs (DHA), Bern (CH)

Europe has staked its future prosperity and social well-being on its ambition to become the world's leading knowledge economy. In order to achieve this it must improve its performance in each dimension of the "knowledge triangle" of education, research and innovation. In particular, this involves building better linkages between each of these domains and between the actors involved: the leading edge universities and research institutions and the most visionary enterprises.

In my capacity as European Commissioner for Education and Culture, I have sought to promote dialogue and interaction between these worlds which have, in Europe, too long tended to stay apart. I set out the message in a 2006 communication on modernising higher education that Europe's universities have a potentially huge role to play in driving the knowledge economy and that it will help them greatly to do so if they link with enterprises to create new curricula and open new research fields. More recently, in 2008 I set up the EU University-Business Forum as a space for the two sides to air their specific concerns and to create the ground for joint working.

Most importantly, I launched in 2006 the idea of creating a European Institute for Innovation and Technology (EIT) to be a centre where, addressing frontier, vital fields of knowledge, the best European minds could work together to deliver excellent education, ambitious programmes of research and, ultimately, life-changing innovations. The key underlying principle of EIT is partnership between Europe's centres of excellence, wherever they exist. I'm happy that EIT has moved rapidly from being an idea to reality, with the first generation of operational entities, the Knowledge and Innovation Communities (KICs), starting work in 2010.

As I look at the GENNESYS study, I find strong echoes of the objectives which I have sought to promote in these different initiatives. GENNESYS is opening up an area of frontier knowledge which holds the capacity to impact very strongly and positively on our future. It is built on partnership between leading institutions drawn from the worlds of academia, research and enterprise. And it has declared its goal of using the knowledge generated to address real needs, of turning knowledge into innovation.

I want to take this opportunity to salute the approach taken and the important work done. Europe needs more ventures like GENNESYS. May the spirit of enquiry and partnership which it has launched continue and flourish.

Ján FIGEL'

European Commissioner for Education, Training and Culture, Brussels (B)

GENNESYS is a wonderful initiative; it not only presents a thorough overview of the nanomaterials science and technology spectrum worldwide but it also clearly highlights the research needs which Europe needs to undertake during the next 10 to 20 years if it is to achieve invaluable breakthroughs in this fascinating field of nanomaterials – breakthroughs which will enable Europe to place itself amongst the top-ranking competitive industrial regions in the world. Compiled by the Max Planck Institute for Metals Research in Stuttgart with contributions from many leading scientists in Europe, GENNESYS is not just about reporting research; its primary intention is to provoke a discussion of all issues related to nanomaterials science in Europe, including such issues as social and political awareness, research infrastructure priorities, and the uptake of new technology by industry.

In our dynamic and competitive world, we must meet contemporary demands for a better quality of life, whilst reducing our dependence on natural- and energy resources and the burden we place on the environment. As an interdisciplinary field, the domain of nanomaterials science will act both as a basis as well as a force of momentum for a great number of future discoveries, underpinning many of the technologies which are essential for their development and success in areas such as nanoenergy, nanomobil, nanochemistry, nanoelectronics, nanobiology, nanomedicine, nanosecurity, and so forth. Tomorrow's technology cannot be developed by simply extrapolating our current knowledge. There is no escaping from the fact that the breakthroughs necessary for achieving these goals can be achieved solely through substantial investment in fundamental research and its associated research infrastructures.

It is our firm conviction that the proposed GENNESYS European research centres, in joining forces, present an excellent blueprint as to how European centres of excellence can be created in a new and modernised way – centres which will be seen to attain a status of global leadership which will benefit the whole of Europe. GENNESYS will have a great impact in the future successes of the European large test facilities, providing scientists and industrialists of the new member states with the opportunity to participate in these fore runners of research. Moreover, this initiative presents industry with the necessary challenge of realising new ideas for technology transfer. In addition, GENNESYS will be an excellent school for students and young scientists, preparing them for brilliant careers. Finally, GENNESYS is in full line with the EERA-initiative, and it is a great example in which the cooperation of all European research efforts will be foreseen.

GENNESYS is addressed to all nanomaterials scientists and scientists from related science disciplines in Europe, as well as regional, national and European policy-makers and managers in industry. It serves as a call to European politicians to upgrade investment into GENNESYS science- and technology centres of excellence to a level at least comparable with that in other industrialised countries, notably the US and Japan, so that European industry can remain competitive well into the future. Only then can we pass on a culturally, scientifically and economically flourishing Europe to future generations.

GENNESYS is a great initiative and will become the motor of the nanoscience and nanotechnology community in Europe. For this reason, we believe that GENNESYS should be supported wholeheartedly by all policy-making bodies and research institutions throughout Europe.

Philippe BUSQUIN

Member of European Parliament, Committee on Industry
External Trade, Research and Energy (ITRE)
Chairman of the Scientific Technology Options Assessment Panel (STOA)
Former European Commissioner for Research, Brussels (B)

Jerzy BUZEK

Member of European Parliament, Committee on Industry, External Trade, Research and Energy (ITRE), Brussels (B)

Today, society is faced with the challenge of globalisation. This particularly affects Europe's industry, economy and academia. With conventional manufacturing dominated by developing economies, the future of industry for Europe must rely on its capacity for innovation, rather than on improving existing technologies and products. We live in a knowledge-based and information driven society in Europe. We are currently witnessing worldwide competition to establish the very best centres of excellence to generate new knowledge and technologies: interacting with these centres is a must for European industry to gain global leadership.

This is why the GENNESYS initiative to establish Europe at the forefront of nanomaterials is extremely important for our future economic prosperity. The field of nanomaterials is one of the fastest growing and most important scientific developments in the last half-century and European industry has recognised its significance to many industrial sectors in Europe. In view of its novelty and complexity of the technology at the atomic level, the importance for industry to engage in partnership with the scientific community is obvious, requiring the best brains and the most advanced facilities.

COST – the acronym for European CO-operation in the field of Scientific and Technical Research – was the first and is the widest network to coordinate nationally funded research activities. Established by a Ministerial Conference of 19 European states in November 1971, COST is at present serving the scientific communities of 35 European countries and is a cornerstone for the development of the European Research Area. The more than 200 research COST Actions are coordinated by the COST committees in nine scientific domains. One of these nine scientific Domains is "Materials, Physical and Nanosciences" and in October 2006 COST organised in Brussels a "European Forum on Nanosciences" in cooperation with the European Commission, the European Science Foundation, the European Parliament and the ERA-NET Consortium on Nanosciences. The recent increased financial support for COST established in the Seventh Framework Programme makes COST a very interesting opportunity for the European scientific community to cooperate in selected topics in the field of nanosciences and nanotechnologies.

Francesco FEDI
Chairman of the EU-COST Senior Officials Committee, Brussels (B)

This European foresight study has been carried out during the last five years chaired by the Max Planck Institute for Metals Research in Stuttgart. The GENNESYS document is a worldwide unique reference document, as it has successfully achieved to develop a sustainable action plan for the development of nanomaterials and nanotechnology in Europe that underpins the various technology roadmaps with the necessary knowledge base on the nano level. Knowing how diverse and complex this field is, I can only congratulate all authors and contributors to this study for making this truly remarkable effort.

The conclusion and recommendations of GENNESYS go significantly beyond any other European strategy in nanoscience and nanotechnology and can solve several of the most vexing problems we currently have, if we turn these ideas into reality. One of the key problems is the multiple fragmentation of efforts in Europe which goes across scientific disciplines and sectors and across the European member states. Also very high up in the "European To-Do-List" are the strategic integration of the existing research infrastructure and the development of a interdisciplinary education strategy for the nanomaterials scientists and engineers we need in order to tackle the problems of tomorrow.

I specifically welcome the GENNESYS recommendation to create European science and technology centres of excellence for the targeted development of novel nanomaterials in order to solve most urgent problems of our society, as new materials for environmentally friendly energy concepts. The Max Planck Society already established successful research structures that now may serve as inspiration to these new European centers.

So, I am extremely pleased with the final results and I would like to thank the Max Planck Institute for Metals Research for embarking into this effort and for pushing it to this fine result.

Martin STRATMANN
Vice President of Max-Planck-Gesellschaft (DE)

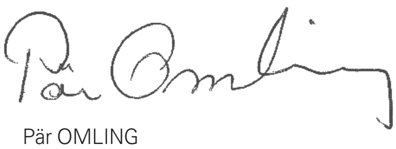
More than 20 years ago, I switched my scientific interest to nanotechnology, nanoscience and in particular to nanomaterials. At that time, the field of nanomaterials was rather small, narrow and unknown, but unexplored and, therefore, challenging. The developments have, however, surpassed most of our early predictions of the future and today nanomaterials is a broad, advanced, but still challenging, field of science.

The present study, GENNESYS is an impressive and comprehensive documentation of the status and foreseen future of nanomaterials. It is outstanding in its coverage, beautifully presented and gives easy-to-understand descriptions of the different nanomaterial technologies research issues and challenges of today. It will most certainly become the reference work for students at universities, as well as for professionals in the field: professors, research managers, academic researchers and industrial researchers. In the attempts to make Europe competitive with other major players in the field like US and Japan, GENNESYS is a good basis for strengthening the competition, collaboration and, when needed, coordination of the sometimes scattered nanomaterials research in Europe.

In particular, I find the ambitious approach to cover the whole value chain from basic research, through engineering and technology, to industry and the required infrastructure, and to implications for society including ethical and environmental implications, very impressive. It is rare to find such a comprehensive description of a field and its present challenges, and it is a great pleasure to read it.

The results of the GENNESYS project are many new ideas, guidance for possible scientific breakthroughs, and important recommendations. Of particular importance for the European science community are the proposals to create new institutes or centres for nanomaterial research. In Sweden this has e.g. been discussed in relation to plans for large research infrastructures such as synchrotron and neutron facilities. Another interesting recommendation is the creation of a new College of nanomaterials. The project also highlights breakthroughs and future applications of nanomaterials in fields such as energy technology, global climate change, security and safety as well as for cultural heritage.

GENNESYS is a very impressive overview of the nanomaterials research and is also an ambitious forward look covering the decades to come. Because of the inclusions of all parts of the research chain – academia, industry and society – it forms a good basis for informed discussions on priorities, opportunities, strategies, limitations as well as potential risks. The GENNESYS study is therefore a most welcome document which most likely will have a great impact on the European research agenda.



Pär OMLING

Director General of the Swedish Research Council (SE)
Former President of EUROHORCS

Nanomaterials science requires a whole new mindset to understand the possibilities that these materials potentially offer to society. There is a simple analogy that I find useful. It is the comparison between the freedom of an individual person walking on their own compared with a well-drilled army marching in unison. For many years we have dealt with materials as agglomerates of atoms. Even if randomly packed, the average properties of a bulk assembly are relatively easy to determine although there is still ample scope for new bulk materials to be developed. However, when we are down at manipulating individual atoms, there are a whole new set of characteristics that come into play which we are still at the start of exploring.

X-ray and neutron sources can give us atomic information both at the electron and nuclear level. They have provided amazing breakthroughs in structural biology, magnetic materials and in our understanding of chemical processes, for example. The worldwide investment in synchrotrons has blossomed since the first dedicated synchrotron was commissioned at Daresbury in the UK over 25 years ago. Upgrades to both the European neutron and high energy x-ray sources in Grenoble are being pursued to ensure they will be fit for purpose for the next decades. Proposals for a next generation neutron spallation source are being actively championed in Europe and similar facilities are coming on stream in Japan and the USA.

Ultimately, we need to observe the dynamics of nanomaterials both as they are processed and as they are applied. X-ray free electron lasers offer the promise that we can directly observe atom to atom interactions. The LCLS in California is now performing and the agreement to build the European XFEL is on the verge of being signed by several countries. Early results from the FLASH facility in Hamburg are demonstrating the effectiveness of resolving processes at the few tens of femtosecond time period. With the higher energy machines, watching movies of atoms and molecules interacting is a very exciting possibility. Many of the potential applications are outlined in this book. While the majority will be in entirely new fields, we should not overlook the application of these machines to observe the first elements of corrosion or bio-fouling for instance. A time-resolved understanding of the first few microseconds of these reactions could well lead to significant cost savings in many industries in addition to improving safety.

It is also important to realise that alongside these hardware developments, petascale nanomaterials modelling and simulation will be in place and gridlinked to the facilities. Both will inform each other possibly in real-time. A key question is, just how will researchers control such interactions and how will they deal with the data deluge? I firmly believe that there needs to be a new paradigm shift in the way new researchers are trained if we are to maximise the benefits of these interactions.

The future of this field is exceptionally bright and many treasures lie before the researcher at the start or midway through their career. This work of GENNESYS is a "Tour de Force" and is a monumental milestone in the future of all things nano.

John WOOD

Former Chief Executive of the Council for the Central Laboratory of Research Councils, Chilton (UK)
Former Chairman of the European Strategy Forum on Research Infrastructures, Brussels (B)
Professor at Imperial College, London (UK)
Chairman of EC Research: ERAB, Brussels (B)

Today, we must embrace the fact that society is being faced with the challenge of globalisation. This particularly affects Europe's industry, economy, and academia. With conventional manufacturing increasingly being pursued by developing economies, future European industry must rely on its capacity for innovation, in the sense of breakthrough innovations as well as the improvement of existing technologies and products. We live in a knowledge-based, information-driven society and are currently witnessing worldwide competition to establish the very best centres of excellence to generate new knowledge and technologies.

It is for this reason that the GENNESYS initiative, which aims to establish Europe at the forefront of nanomaterials, is of such importance to our future economic prosperity. The field of nanomaterials is one of the fastest growing and most important scientific developments in the second half of last century and European industry has recognised its significance to many industrial sectors in Europe. In view of its novelty and the complexity of technology at the atomic level, the importance for industry to engage in partnership with the scientific community is obvious, requiring the best brains and the most advanced facilities.

The opportunity for science/industry partnerships envisaged by GENNESYS is warmly welcomed. Moreover, the spin-off of science to technology will pave the way for close collaborations between industry and Europe's large scientific test facilities, such collaborations being crucial to the commercial success of nanomaterials. The proposed "GENNESYS" European centres of excellence will provide access for industry to advanced synchrotrons, neutron sources and other facilities in order to help tailor materials, optimise processing conditions both in-situ and non-destructively, and characterise their behaviour in service. GENNESYS presents the unique opportunity for talented scientists from both industry and research to work side by side to specify industry's requirements and assist in the development of production processes and manufacturing techniques that can be readily adopted by industry.

GENNESYS will benefit many industrial sectors vital to securing Europe's future. Nanomaterials will act as a driver for discovery and innovation, helping to maintain Europe's position in the field of leading-edge technology for many years to come. Europe should join together and support the GENNESYS initiative. The fostering of collaborations between regional, national, and European institutions, industry and funding agencies will prove crucial in building a strong base for European success.

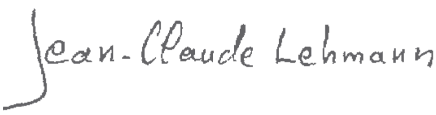
GENNESYS offers great potential to industry, presenting it with the opportunity to enter into a partnership with science in the new centres of excellence. These centres of excellence represent a new kind of technology transfer that will benefit all materials and industrial sectors. In addition, the centres will serve as an excellent training ground for future recruits to industry.

In order to promote the GENNESYS initiative in European industry, familiarise the industrial researcher with the potentials of large test facilities in the broad field of nanomaterials, and to optimise large test facilities' capabilities and uses for industry, industrial federations and national technology academies may play a key role under the umbrella of national governments, the European Commission, and international organisations.

In conclusion, the GENNESYS initiative should be applauded for its plans to strengthen the bonds between the nanomaterials science community and industry, as it offers an efficient way to perform experiments at the large test facilities, within a European framework. The GENNESYS research centres will become ideal think-tanks for industry in the nanoworld and these advanced analytical test facilities will be vital tools for discoveries and innovations.

Rüdiger IDEN

Senior Vice President, BASF S.E. (DE)
Co-Chair of the European Technology Platform for Sustainable Chemistry (ETP SusChem), Ludwigshafen (DE)



Jean-Claude LEHMANN

Former President and Current Member of the "Académie des Technologies Française", (NATF), Paris (FR)
Former Vice-President of Research and Development, Saint-Gobain, Paris (FR)

As Chairman of ESFRI, and as a materials scientist, I welcome the publication of the GENNESYS foresight study as a major contribution to the development of a coherent and effective policy in research and research infrastructures in Europe. The ESFRI action, to help the European countries and the European Commission in integrating their efforts to reach a world level competitiveness, is greatly enhanced in all those fields where the scientific communities are capable of developing and proposing science-based foresights and roadmaps. These proposals give strong and useful support to policy makers, helping them to invest the limited available resources in the most effective way to increase the capability of European research.

The development of nanoscience and nanomaterials research in Europe is critically dependent on the availability of instruments for the analysis and synthesis of materials, from metals to biological materials, at levels and volumes not normally available in university and research institutions. This requires a number of multipurpose research infrastructures, service-oriented and capable of offering excellent support to researchers, with free access open on the basis of quality only. These infrastructures also act as multi-disciplinary and international meeting places, opening new and important opportunities for researchers and technicians coming from different environments.

Materials sciences are eminently multi-disciplinary, and the research environment is very important to allow the collaboration with the right mixture of specialised knowledge which may lack in smaller groups. The synchrotron and laser, as well as the neutron beam based laboratories, each serving hundreds to thousands researchers every year, are meeting places of this kind. However, they should not act in isolation but need to be integrated in a larger network of facilities offering several complementary features and specialised laboratories, allowing the control on the needed extensive ranges of phase parameters, like pressure, temperature, magnetic fields etc., or integrating the photon and neutron probes with other complementary probes like in electron microscopy and with nano-foundries to support frontier research in novel nanomaterials.

The availability of an integrated foresight and landscape, as in the GENNESYS report, allows to understand and explain, at policy level, how it is possible to develop multiple partnerships and joint projects between various different laboratories, building an integrated "overall infrastructure" in Europe. It will be very important that the scientific communities involved in materials sciences and in the nanoscience activities become vocal and organised at a European level on a more long-term basis, to develop a reference capable of suggesting priorities and choices at the EU policy-making level.

Carlo RIZZUTO

President of ESFRI (B)
President Sincrotrone Trieste (I)

GENNESYS is most welcome; it gives an excellent overview of the large spectrum of nanomaterials science and technology, pinpoints and prioritises the important areas for future research and highlights the role of synchrotron radiation and neutrons in helping to achieve breakthroughs in nanomaterials science and technology.

A valuable roadmap has been developed to bridge the contacts with industry; it enlightens the importance of many areas of nanomaterials in health and industry which wait for breakthroughs: medicine and foods; energy, transport and environment; safety and security etc. where nanotechnology is in its infancy. This strategy study does not only assist policy-makers and funding agencies in their decisions for targeted funding, it will also help research- and industrial managers to adjust their research strategies and directions. In addition, it will be a useful tool for researchers and students to select topics which guarantee success in their studies/work.

Nanomaterials science and technology has a worldwide interest; it will affect the welfare and play a key role in the future economy. It encompasses a broad field of applications and offers enough possibilities for all research and development laboratories in the world to take part in groundbreaking research. In addition, it is a most complex and new topic which demands for an international collaborative effort in order to reach scientific breakthroughs, to promote industrial innovation, to evaluate risks of global consequences and to establish nanomaterials standards for world markets.

GENNESYS is a wonderful European initiative of which it is hoped that it will become the nucleus for international collaborations in this important domain of nanomaterials science between laboratories, research institutes and large test facilities in Asia, the America's and the whole world. GENNESYS may also have an impact in developing countries where nanomaterials may have an impact in the areas as agriculture-, food, energy, water treatment, drugs delivery systems etc.

Nanomaterials offer challenges for a world common education philosophy in this new materials field; it contains elements which have scope for an international education programme, providing opportunities for exchange programmes for young students and scientists between laboratories worldwide. GENNESYS is a unique initiative in the sense that it sets out a possible education/research infrastructure for worldwide education in the field of nanomaterials.

GENNESYS should receive the attention and the involvement of governments all over the world as well as international organisations: UNESCO, the United Nations, International Energy Agency (IEA), and OECD. These organisations should foster worldwide collaboration in this new and evolving field.

Japan has also sizeable nanomaterials programmes of which NIMS (National Institute for Materials Science) are coordinating the activities and "SPRING8" has great potentials for synchrotron radiation. In this context, the GENNESYS initiative is a great idea and I wish that the ambitions for international collaborations will be realised and NIMS will be a strong supporter.

Teruo KISHI

President of the National Institute for Materials Science (NIMS), Tsukuba (JP)
Former Vice President of the Japan Science Research Council, Tokyo (JP)

Europe operates some of the best large-scale scientific facilities (LSF) in the world – with an increasing impact on nanoscience and nanotechnology. Most notably, synchrotron and neutron sources produce world-class scientific contributions in many domains relevant to nanomaterials such as physics, chemistry, biology, and materials science. The GENNESYS initiative can put Europe at the cutting edge of nanoscience and nanotechnology by an effective and coordinated use of these facilities.

The impact of synchrotron and neutron techniques on nanoscience will rapidly expand in the next decade: they will discover new phenomena, probe the secrets of nanomaterials, and yield general results that will strongly influence future technologies. The behaviour of nanomaterials will be examined at unprecedented levels of complexity and nano-microscopic control. The results will help nanoscience and nanotechnology to move beyond fundamental research and produce materials and systems that will impact our everyday life. This evolution requires a better understanding of electronic and optical phenomena, complex assemblies of atoms and multicomponent nanomaterials, non-equilibrium phenomena and nanobiology mechanisms; the corresponding technological frontiers ranging from nanoelectronics to structural nanomaterials and nanomedicine.

Broadly speaking, synchrotron and neutron facilities will enable researchers and industries to investigate increasingly complex and diluted nanosystems with increasingly smaller dimensions and lower cross-sections. The use of such facilities, however, is not immune from problems. They are large, complex and rather expensive. Furthermore, progress in nanomaterials research depends on the ability to synthesise, characterise, manipulate and control nanomaterials from the atomic level to bulk structures. The necessary equipment becomes increasingly sophisticated and requires high-level human resources in scarce supply. The corresponding investments often put these activities beyond the capabilities of individual companies and academic institutions.

GENNESYS can provide the solution for these problems with a strategy based on large-scale facilities and centres of excellence. Large national facilities are indeed ideal hosts for European-level GENNESYS centres for nanoscience and/or technology.

This approach is particularly important for the scientists and industries located in less-favoured regions. At present, most large-scale facilities are concentrated in a subset of European countries. The integrating activities supported by the European Commission are very successful in opening these instruments to scientists from all over Europe, with a selection based on merit and no financial discrimination. The most positive consequences are the increase in scientific output of less-favoured countries and the elimination of the need to emigrate. These results are specifically important for a competitive area such as nanoscience and nanotechnology.

The GENNESYS strategy can become reality if supported by the necessary political and funding decisions. The financial resources required to equip and support major facilities at specific European locations can be provided by exploiting a significant portion of the funding for nanomaterials research by regional, national and EU agencies. The centres so established will become contact places for experimentalists and theorists, for scientists from different disciplines, and for harmonising the educational and research role of universities and national laboratories to industrial needs. These exciting breeding grounds will certainly attract many of the world's leading scientists.

In summary, the GENNESYS strategy will boost the role of European large-scale synchrotron facilities in nanoscience and nanotechnology by making them more user-friendly, by welcoming scientists from a variety of disciplines and creating additional strong links with industry. It is, therefore, a wise and effective strategy which deserves full support.

Giorgio MARGARITONDO

Vice-President for Academic Affairs, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne (CH)
President of the Council: 'European Integrating Initiative for Synchrotron Radiation and Free Electron Laser (IA-SFS), Brussels (B)

EDITOR'S NOTE

We thank all authors, contributors and experts who made this document possible.

GENNESYS is a strategy document and contains no references to original publications.

All external figures which are used in the document are marked accordingly.

The input of very many experts has been merged together to this document. It was unavoidable that not all information could be integrated. We hope for understanding.

We are most grateful to Paulien Staal for all the editorial work and to Hoa Phuong Nguyen for her help during the last phase of the preparation of GENNESYS.

We thank the Max Planck Society for the continuous support of this project.

Helmut Dosch
Marcel H. Van de Voorde

Max-Planck-Institut für Metallforschung

1. INTRODUCTION

AUTHOR: H. Dosch
[Affiliation chapter 12]

1.1. WHAT IS NANOMATERIALS SCIENCE AND NANOTECHNOLOGY?

Nanoscience and nanotechnology are based on the control of the structure and function of materials on the nanometre scale, i.e. on the scale of one billionth of a metre. The gateway to nanoscience and nanotechnology has been opened more than 100 years ago, when W.C. Röntgen discovered the x-rays which allowed us to unravel the nanoscale structure of matter and when Planck, Heisenberg, Schrödinger, and Einstein developed the language of the nanocosmos: quantum mechanics. During the last 100 years, a truly breathtaking scientific and technological development has taken place, which can be illustrated by quoting three scientists:

1900, Ernst Mach: "Atoms cannot be perceived by the senses. They can never be seen or touched, and exist only in our imagination."

1950, Richard Feynman: "The principles of physics do not speak against the possibility of manipulating things atom-by-atom."

2000, Sir Richard Smalley: "Nanotechnology is the art of building devices at the ultimate level of finesse: atom-by-atom."

Nanotechnology is a collective term for a set of technologies, techniques and processes – effectively a new way of thinking – rather than a specific area of science or engineering. Just as electronics and biotechnology have created their own technological revolutions, nanotechnology will have a similar impact; in some areas sooner rather than later. Often referred to as 'convergent technology', nanotechnology is an interdisciplinary ensemble of several fields of the natural sciences that are in themselves highly specialised. The ultimate atom-control of the nanosize and shape as well as of the nanogeometry of novel materials and materials architectures will open up a third dimension on the Periodic Table.

Only few industries will escape the influence of nanotechnology. Faster computers, advanced pharmaceuticals, controlled drug delivery, biocompatible materials, nerve and tissue repair, surface coatings, better skin care and protection, catalysts, sensors, telecommunications, magnetic materials and devices – to name but a few of the areas where nanotechnology will have a major impact. In effect, nanotechnology is a radically new approach to manufacturing. It will affect so many sectors that failure to respond to the challenge will threaten the future competitiveness of a large part of the economy.

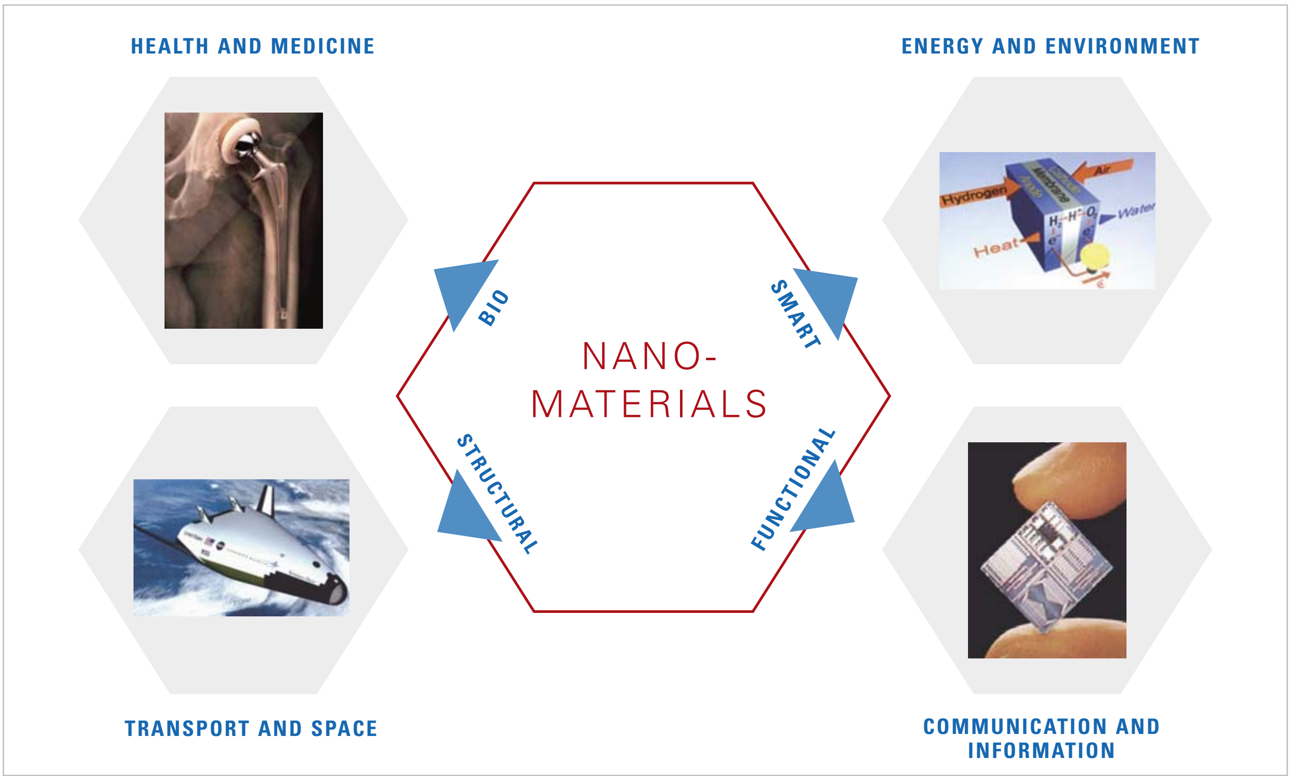


Fig. 1.1: The impact of nanomaterials in industry and society.

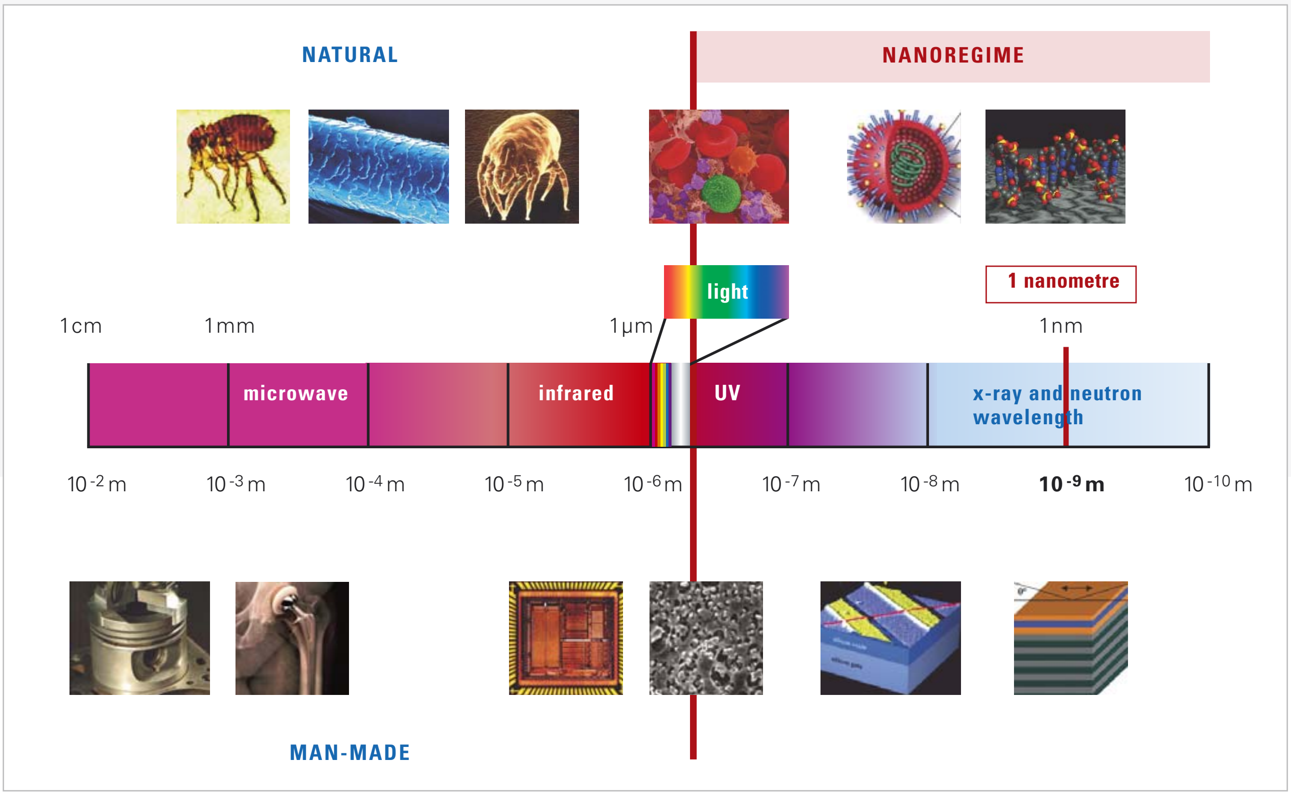


Fig. 1.2: Typical length scales in current and future technologies.

1.2. NEW MATERIALS FOR NEW TECHNOLOGIES

Advanced materials are a prerequisite for all major research and development areas and for all key technologies ranging from information and communication, health and medicine, energy and environment, to transport and space exploration. Sophisticated materials and materials systems with novel properties and unheard of performance will have to be conceived and designed in the decades to come. This will be imperative if the European high-tech industry is to remain competitive and if a high standard of living is to be guaranteed for the European citizen in the 21st century.

The development of the materials of tomorrow will make increased use of new nanoscience concepts, i.e. the design of artificial material structures within the ultimate limit – atom control. New nanofunctions will be created by the control of size and shape of the nanoparticles as well as by the controlled interactions between them across tailored interfaces. In this way, future materials research will open up a new dimension in the periodic table allowing new materials functions beyond the properties tagged by nature to the elements. These future visions of nanomaterials science bearing on the virtually infinite possible materials combinations and on the resulting emergent phenomena have been anticipated by Richard Feynman's "There is plenty of room at the bottom" and Phil W. Anderson's "More is different".

It is expected that new nanomaterials will find their way into almost all future technologies: New nanoparticle-reinforced and light-weight materials will be used for transport technologies; new storage media based on nanolayers and quantum dots will revolutionise information

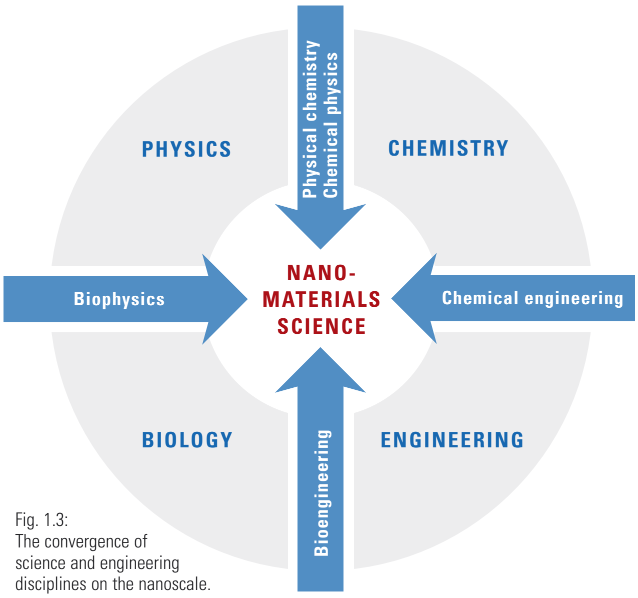


Fig. 1.3:
The convergence of science and engineering disciplines on the nanoscale.

technology; new materials based on nanoparticles will be employed in catalytic reactors; new pharmaceutical nanomaterials will serve in drug delivery, and new charge separation materials will enhance the performance of future batteries and fuel cells, to name but a few examples of new applications.

Future nanotechnology will be enabled by enhancing fundamental research in the critical areas of nanomaterials synthesis, nanomaterials analysis, and nanomaterials modelling. In all these areas there are major challenges to be met and barriers to be overcome. More specifically, it is necessary that we:

- Achieve a much better control of the size and shape of the primary nanoparticles in order to exploit their full potential ("precision synthesis");
- Develop a new level of analytical capability for the in-situ and destruction-free characterisation of nanomaterials and nanodevices under the relevant operating conditions as well as with the highest resolution and sensitivity;
- Develop a detailed microscopic understanding of how a given artificial nanoarchitecture and its properties are related.

The development of new nanomaterials will no longer be limited by our resources, but instead by our knowledge. The design of such "knowledge-based materials" requires new concepts which will *inter alia* be based on two interdisciplinary strategies:

• **"Interdisciplinarity I":** The expert input from the field of physics, chemistry, engineering, and biology is required. This poses a challenge both for future research structures, as well as for the future training of young scientists who not only have to remain experts in their own field, but must also improve their literacy in neighbouring fields.

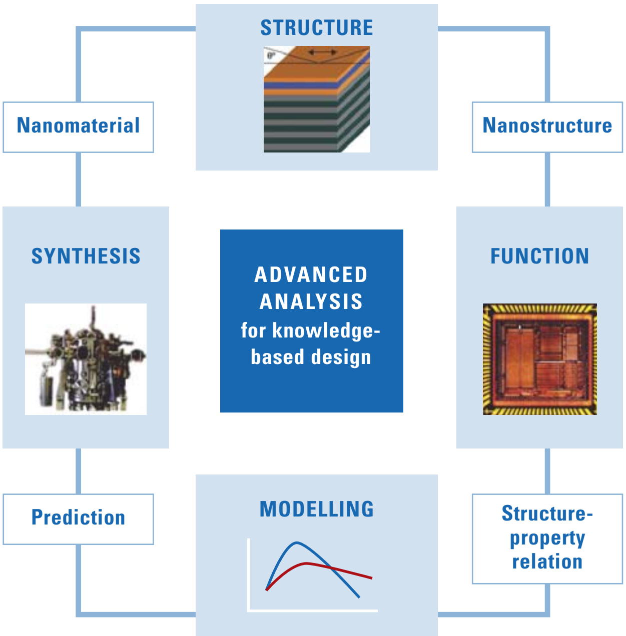


Fig.1.4: Role of advanced analysis for nanomaterials science and nanotechnology.

• **"Interdisciplinarity II":** It is mandatory that the experts in materials synthesis collaborate intimately with the experts in materials analysis, materials functions and with experts in materials modelling. It is only with the detailed knowledge of the microscopic structure of the grown nanomaterial at hand that a microscopic structure-function relationship can be obtained. This knowledge can then be cast into theoretical models which carry sufficient predictive power to modify the synthesis parameter in the most promising direction.

It is apparent that our future capabilities in nanomaterials analysis will play a key role for the advancement of nanomaterials and nanotechnology. New types of interdisciplinary materials science centres must include a new level of analytical capability. Such new "Science Centres" will integrate new nanomaterials synthesis capabilities with an in-situ and non-destructive analytical infrastructure of the function, performance, and failure behaviour of nanomaterials and nanodevices as well as with the necessary computing capacities.

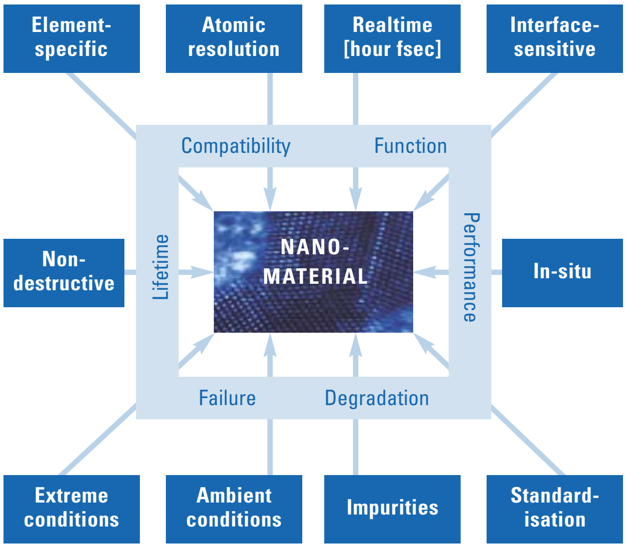


Fig.1.5: Future analytical need for the development of nanomaterials.

1.3. FUTURE ANALYTICAL CHALLENGES

The advanced analysis of nanomaterials is the future enabling technology for the development of novel materials and nanodevices. Detailed knowledge of the chemical, electronic, and magnetic structure of nanomaterials is a prerequisite to tailor their functions in a controlled way, and to develop microscopic models with predictive power. This includes subtle structural details, such as strain profiles across interfaces with picometre resolution, impurities and composition variations with single atom detection capabilities, or the precise separation of spin and orbit contributions to a local magnetic moment. In the next two decades, the need from nanoscience and nanotechnology to obtain these important microscopic insights into their nanomaterials and -devices in-situ, in a non-destructive way and under industrially and environmentally relevant conditions will increase exponentially.

While the traditional analytical tools of the materials scientist, i.e. transmission electron microscopy together with routine spectroscopy and routine x-ray and neutron diffraction (i.e. power diffraction and small angle scattering) have been very efficient for traditional materials research, these tools cannot meet the aforementioned challenges of tomorrow's nanomaterials design.

1.4. THE EUROPEAN SYNCHROTRON RADIATION AND NEUTRON FACILITIES

The European Synchrotron Radiation and Neutron Facilities provide an exquisite analytical potential for the detailed analysis of nanomaterials. Starting as research laboratories pioneering the use of neutrons and synchrotron radiation, they have developed into dedicated, user-friendly facilities offering their clever analytical solutions to external research groups.

X-rays and neutrons are generally known to be bulk-sensitive techniques that provide "average structural information" for a given material. However, sophisticated new concepts, developed at these facilities in the past twenty years, have completely changed this situation. New diffraction and spectroscopy schemes, new focusing optics, new imaging and microscopy concepts having been worked out along with the development of more brilliant and more powerful sources now allow for a revolutionary new analytical access to nanomaterials.

Europe's synchrotron radiation and neutron facilities have developed a European network simultaneously ensuring synergetic development of key technologies for the future demands in advanced analysis as well as a coordinated user service.

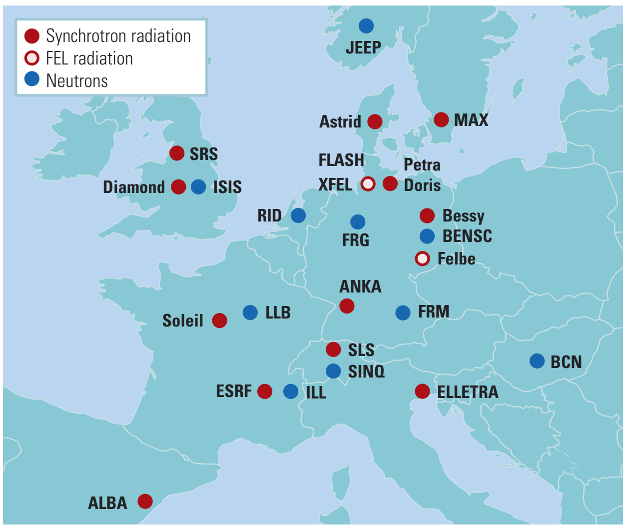


Fig. 1.6: European research infrastructure for the fine analysis of matter.

1.5. GENNESYS: A NEW NANOMATERIALS STRATEGY FOR EUROPE

In the last two decades, the synchrotron x-ray radiation and neutron facilities in Europe have developed a highly sophisticated and reliable analytical technology which carries the potential to meet the future analytical challenges for the development of new nanomaterials and the advancement of nanotechnology. It is thus rather surprising that the two scientific communities, the nanomaterials laboratories on the hand and the large scale facilities on the other hand, have developed rather independently and are thus largely unaware of each other's existence.

At present, the materials science and synchrotron radiation and neutron communities carry out research virtually separately. Synchrotron radiation and neutron facilities have developed revolutionary new ideas and experimental schemes to characterise nanomaterials, nanophenomena, and nanoprocesses in a most sophisticated manner, but they are largely unaware of the trends and needs in the nanolaboratories. Likewise, most of the nanomaterials and nanotechnology scientists have only little information on and limited knowledge about the enormous analytical potential provided by the synchrotron radiation and neutron facilities and its use for solving their problems. It is apparent that this fragmentation of efforts has to be overcome, if Europe wants to stay competitive with the nanoscience and nanotechnology development in the USA and in Asia. It will become an important task of European science policy to set up efficient European research structures leveraging the current and future potential of the European large scale facilities for synchrotron radiation and neutron science for the development of nanomaterials and nanotechnology.

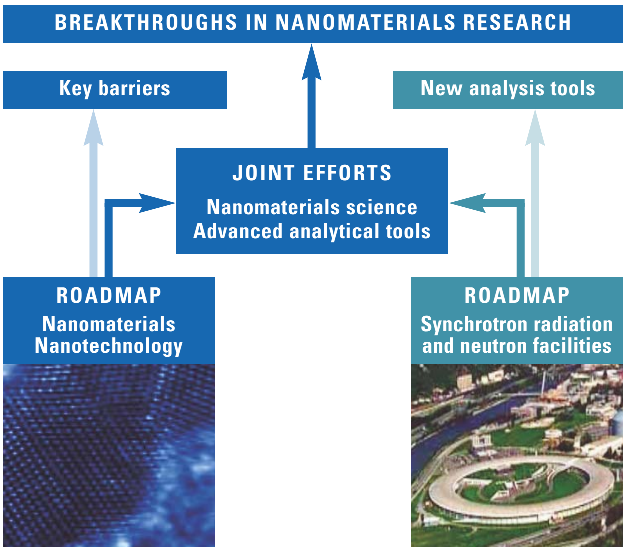


Fig. 1.7: The GENNESYS objective.

The Grand European Initiative on Nanoscience and Nanotechnology using Neutron and Synchrotron Radiation Sources (GENNESYS) has been initiated to achieve this goal and to develop new European research strategies to facilitate joint efforts between the nanomaterials science and the European large-scale facilities for the advanced analysis of materials in order to overcome the key barriers in the development of nanomaterials and nanotechnology that are already visible on the horizon.

This White Paper gives a condensed report on the major findings, conclusions and recommendations of the GENNESYS project for the various fields of nanoscience and nanotechnology. Several general problems have been disclosed by the GENNESYS task forces in current materials science efforts:

- **Lack of public awareness:** While all future technologies rely on the precise and dependable performance of specialised materials, the role of materials science is often not appreciated by the public because its activities generally take place in the background.
- **Fragmentation of materials research efforts:** Materials science in Europe is severely fragmented, as research is often performed within isolated and subcritical efforts.
- **Communication gap between nanomaterials science and large-scale facilities:** Nanomaterials research is frequently based solely on lab-based research tools and researchers are generally unaware, or cannot access the enormous potential of neutron and synchrotron characterisation techniques. In turn, the management of neutron and synchrotron x-ray radiation facilities only have rather fragile information on the actual and future analytical needs in nanomaterials research.
- **"Horizontal challenges meet vertical structures":** Nanomaterials research is an interdisciplinary ("horizontal") effort integrating the traditional branches of natural sciences and engineering and, in the future, integrating nanolabs and large-scale facilities. In the meantime, national and European funding structures have, however, developed along the traditional ("vertical") lines.

It is hoped that the roadmaps presented in this GENNESYS White Paper will provide a point of reference for policymakers as well as the operators of large-scale facilities. It is envisaged that GENNESYS will serve as a novel and world-wide unique platform for scientists to foster future collaborative, cross-disciplinary research and development, and to stimulate growth in the commercial exploitation of nanomaterials science and technology in Europe.

GENNESYS strives to integrate nanomaterials research, nanomaterials industry, and the European research infrastructure (synchrotron x-ray radiation and neutron facilities) in overcoming the key barriers in the development of new materials for future technologies.

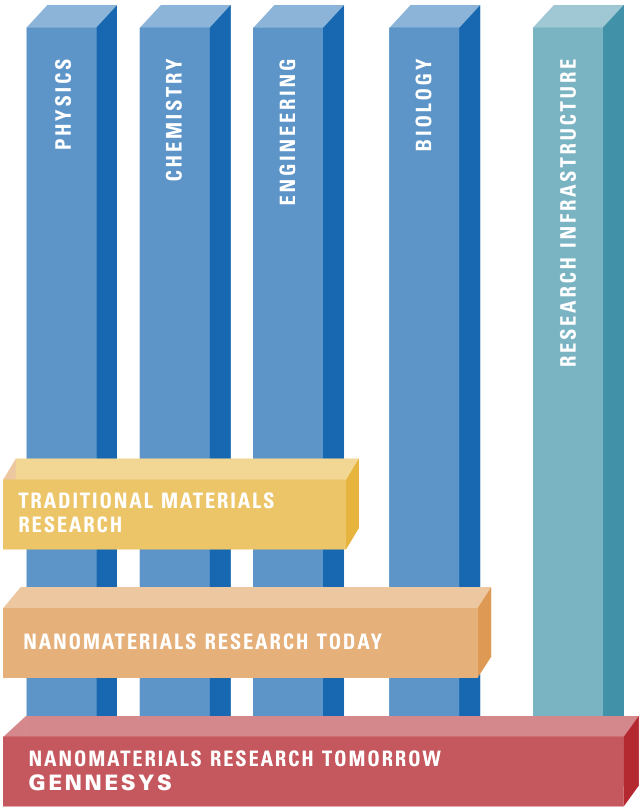


Fig. 1.8: The envisaged future GENNESYS platform.

2. GENERIC CHALLENGES FOR FUNDAMENTAL RESEARCH IN NANOMATERIALS SCIENCE

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Future nanomaterials will create new functions for the applications in future technologies by opening up new dimensions in the periodic table. The control of the number of atoms allows the coupling of materials-inherent microscopic length scales to the size and shape of the nanostructure, thereby evoking new phenomena and functions ("nanoconfinement phenomena"). The control of the geometric arrangement of different elements and systems on a nanometre level gives rise to novel collective phenomena which do not occur in thermodynamic equilibrium ("proximity phenomena"). The number of materials combinations and geometries is only limited by our knowledge and scientific intuition. It is clear though that any future nanomaterials science endeavour will face enormous challenges in all key areas ranging from the synthesis of nanomaterials and nanosystems, the characterisation of nanostructures and the analysis of new phenomena, to the optimisation of their functions and the modelling of nanomaterials properties. Many of these challenges are rather generic (i.e. materials-independent), and it is these challenges which are addressed in this chapter.

2.1. GENERIC CHALLENGES FOR NANOMATERIALS SYNTHESIS

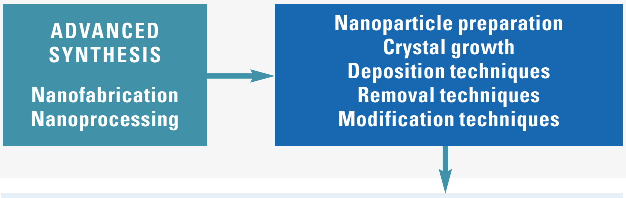
Modern nanomaterials synthesis encompasses a large field of different strategies ranging from the hypercritical drying of primary nanoparticles to the self-organisation of periodic arrays of nanodots. Future nanosynthesis will exploit all states of matter (gas, liquid, solid), all materials classes (metals, ceramics, soft and biological materials) and all synthesis technologies which carry the potential of an atom-controlled assembly. This includes the synthesis of the primary nanoparticles and nanoclusters, the growth of nanocrystals, the deposition of atoms and primary nanoparticles (by sputtering, vapour deposition techniques, MBE, self-assembly, electrodeposition), the controlled removal of material (chemical etching, ion etching, electrocorrosion), and the modification of surfaces and interfaces. A severe boundary condition is that a new synthesis concept should be designed such that it can be scaled up to mass production.

2.1.1. SYNTHESIS OF THE PRIMARY NANOPARTICLES

The precise synthesis of nanoparticles is a prerequisite for the development of high-tech coatings, dispersions and inks, and for the design of selective high surface area materials of consolidated bulk materials with tailored mechanical or magnetic properties.

State of the art

Current processes include aerogel/hypercritical drying, sol-gel processes, gas phase synthesis, (high energy) ball milling, cavitation, polymer-, dendrimer-synthesis, and colloidal chemistry. These processes carry scale-up potential, however, all suffer from the lack of precision and definition in the resulting nanoparticle structures (including size, shape, internal structural gradients) which severely limits their functions. Synchrotron radiation and neutrons have, up to now, been used mainly to monitor the growth of the average size distribution of the nanoparticles by small-angle-scattering techniques. A detailed microscopic picture of the size, shape, and internal structure of the emerging nanoparticles is missing.



KEY CHALLENGES AND GOALS IN SYNTHESIS AND NANOFABRICATION

- New synthesis must include all types of materials (inorganic, organic, bio-)
- Increase reproducibility, precision, control of structural parameter (size, shape, roughness, connectivity, morphology, chemical composition)
- Invent new nanofabrication strategies, develop an in-situ-control of the relevant fabrication parameters
- Synthesis and nanofabrication at the interface to biology
- Synthesis of hybrid materials
- High-throughput screening with spatial resolution in nanoparticle synthesis (particularly for drug production)
- Controlling purity at all synthesis steps
- News ways of self-assembling colloidal particles
- New microfluidic approaches in nanosynthesis
- New interaction between nanosynthesiser and nanoscientists
- Colloidal chemistry: new ways to synthesis in a controlled way non-spherical colloids (rods, pyramids)
- Nanoparticle synthesis (sol-gel gasphase): reduce size variation from 20% to less than 5% (to see quantum effects); use of inverted micelles

Fig. 2.1.1: Overview key challenges in nanosynthesis.

Future challenges

- A further future need is the availability of high-quality crystals with a well-defined size and shape. In order to achieve an improved control on morphology and polymorphism during single crystal growth, a better understanding of the key parameters is mandatory. The potential of biomineralisation as a low-temperature (i.e. low-cost) route to high quality crystals has to be investigated.
- The development of a precision synthesis of nanomaterials and nanocrystals requires the in-situ monitor of structure of the growing nanoparticles in the growth reactor that allows a direct correlation of the growth parameters with the nanoparticle structure. This is a key challenge in all the aforementioned nanoparticle synthesis technologies.
- There is a fundamental lack of microscopic understanding of the initial nucleation process and the subsequent growth process leading to stable nanoparticles. This most important information requires detailed experimental insight into the critical fluctuations leading to metastable nanoparticles, which then serves as input for theoretical models.

Future role of synchrotron radiation and neutron facilities

- Dedicated precision synthesis facilities which include highly specialised synchrotron radiation and neutron diffraction and spectroscopy beam lines providing the in-situ monitor of the relevant structural properties of the growing nanoparticles within the growth reactor are urgently needed.
- Nanoparticle reaction chambers must be equipped with dedicated x-ray and neutron instrumentation that go beyond the small angle scattering regime, but instead cover in real-time a wide range of reciprocal space allowing to reconstruct the internal structure of the nanoparticle during growth. This requires *inter alia* large area detectors with a high dynamic range and rapid data storage, as well as data handling capabilities.
- Time-resolved coherent x-ray diffraction and spectroscopy instrumentation at future free-electron laser facilities have to be joined with the use of a nanoparticle growth reactor in order to access the rapid fluctuations leading to the initial nucleation of nanoparticles.

NEW PRECISION SYNTHESIS

1 NANOPARTICLE PREPARATION
Nanoparticles
Nanopowders
Nanocrystals
Dispersions
Suspensions
Ferrofluids
Inks

2 DEPOSITION TECHNIQUES
Thin films, coatings
Multilayers
Nanostructured functional surfaces
Self-assembled monolayers

3 REMOVAL TECHNIQUES
Nanostructured arrays

4 MODIFICATION TECHNIQUES
Bioactive, catalytic surfaces
Ion implantation
Field emitters
High surface area materials
Consolidated nanostructures

FUTURE NEEDS AND GOALS

(1) Better in-situ control of :
- Size and shape (non-spherical), monodispersity, homogeneity, purity
- In-situ control of internal structure of nanoparticle
- Particle coalescence, particle stabilisation in solution

(2)
- In-situ information on all deposition parameters
- Better control of homogeneity and purity
- Atomic in-situ control of the growth of artificial superlattices
- Combinatorial materials design using deposition techniques

(3) Better understanding and control of the microscopic processes and phenomena during material removal

(4)
- Better in-situ control of all modification processes on the atomic scale
- Achieve pattern formation in materials with <10 nm resolution
- Understand modification during exposure

FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
In-situ x-ray and neutron studies of the microscopic processes during synthesis

(1) Nanoparticle preparation:
- Time-resolved SAXS, SANS with μsec resolution spatial information μ-beam and fully coherent diffraction
- In-situ x/n contrast diffraction
- Time-resolved wide q-space monitoring using large area detectors to control shape and internal structure of growing nanoparticles
- Coherent GID and x-ray topography with nsec-time resolution
- Element-specific x-ray spectroscopy (XAS, x-ray Raman) with 3-D depth resolution
- X-ray FEL instrumentation for ultrafast diffraction and spectroscopy of the nucleation process

(2) Deposition technologies
- Combined beamline providing x-ray and neutron probes and in-situ optical characterisation, AFM/STM and IR spectroscopy
- In-situ neutron reflectometry (H-profiles during implantation, organic and biological materials)
- In-situ spin-resolved neutron reflectometry and off-specular scattering from growing magnetic multilayer
- Dedicated synchrotron radiation beamlines with extended spatial coherence and high intensity for time-resolved GID
- X-ray end-stations for HTP lithography
- HTP synchrotron and neutron beamlines (diffraction, spectroscopy) for combinatorial materials design (implement complementary characterisation techniques)

(3) Removal technologies:
- Dedicated time-resolved x-ray and neutron reflectivity instrumentation
- X-ray GID (using high energy) time resolved x-ray spectroscopy,
- Combined AFM/STM Synchrotron radiation instrumentation highest resolution x-ray diffraction, diffuse scattering, imaging, x-ray tomography

(4) Modification technologies:
- X-ray spectroscopy with sub-μm spatial resolution
- Combined AFM/STM-x-ray beam line (with coherent beam and nm-beam)
- X-ray monitoring of dynamic structural and electronic processes during laser-material interaction on a sub-picosecond timescale with atomic resolution
- X-ray spectroscopy, imaging, energy-dispersive methods

Fig. 2.1.2: Role of synchrotron radiation and neutrons for precision synthesis of nanomaterials.

2.1.2. DEPOSITION TECHNOLOGIES: SYNTHESIS OF THIN FILMS AND MULTILAYERS

Current deposition technologies, such as chemical vapour deposition (CVD), pulsed laser deposition (PLD), and molecular beam epitaxy (MBE), are rather well developed, in particular for inorganic materials, for the growth of thin layers and multilayer devices.

State of the art

Most of these technologies are used in a routine way exploiting empirical knowledge on the best growth conditions (such as flux, substrate temperature, role of surfactants, etc.) Very often the microscopic processes leading to the final structure of the layers are not explored and thus are not under "atomistic" control. In-situ control of the deposition process is done by measuring the mass of the deposited material (quartz balance), optical techniques (ellipsometry) and by RHEED (Reflection High Energy Electron Diffraction).

Key challenges

- Quantitative and easy-to-interpret in-situ control of the emerging structure during deposition, including chemical and magnetic information with atomic resolution and the highest sensitivity for impurities and strain (depth-resolved and laterally-resolved);
- The controlled use of surfactants and the extension of these techniques to organic and biological materials. It is rather unclear, how these strategies can be combined with self-assembly;
- Potential new strategies are self-assembly on chemically or lithographically prepatterned substrates, deposition in the presence of a laser standing wave pattern or DNA-guided synthesis.

Future role of synchrotron radiation and neutron facilities

- Since the parameter space for the different deposition technologies is very large and only little explored, combinatorial strategies should be worked out including non-destructive in-situ analysis exploiting synchrotron radiation and neutrons in order to identify future promising routes for the design of thin films and multilayers.
- X-ray and neutron reflectometry and the associated GID instrumentation combined with complementary optical and magnetic analytical techniques are needed to investigate the evolution of the microscopic structure during deposition. In addition, these techniques are needed to investigate the development of the (desired) properties of the growing layers.

2.1.3. REMOVAL AND MODIFICATION TECHNOLOGIES: NANOSTRUCTURING OF SURFACES

The design of nanostructures by removing materials and modifying existing structures is best known in the semiconductor area (top-down technology). These technologies are slowly approaching, following Moore's law, and the nanometre regime (see Chapt. 5.2.1).

Future goals and needs

Promising areas for the nanostructuring of surfaces are wet (electrified) etching, focused ion beam etching, spark erosion and laser ablation. In order to arrive at a microscopic understanding and control of these techniques, reliable in-situ information on the surface and subsurface structure evolution, strain distribution within a single nanostructure is indispensable.

Future role of synchrotron radiation and neutron facilities

- The development of dedicated nanometre-sized x-ray beams is indispensable in order to access the internal structural and electronic details of individual nanostructures and nanodots and their behaviour during performance.

TECHNOLOGY	NANOPATTERNING OF SURFACES	TEMPLATE-ASSISTED SYNTHESIS OF NANOMATERIALS	MATERIALS FOR NANO-PATTERNS IN IT-SYSTEMS
STATE OF THE ART	E-beam systems available with resolution of ~10nm	<20nm resolution templates produced with EUV-IL	Resists and optical components currently under development
FUTURE NEEDS AND CHALLENGES	Parallel exposure systems for production-compatible throughput with resolution <50nm	Increase resolution, increase exposure area and throughput; develop suitable template and deposition materials	High-sensitivity, high resolution resists
KEY BARRIERS	Photoelectrons, molecular resist structure; statistical nature of material modification during exposure (e.g. shot noise, material granularity)	Pattern formation in materials with <10nm resolution, preparation of high-quality, large-area masks	Preparation of atomically flat interfaces, resolution of chemically amplified resists
RECOMMENDATIONS	Develop and provide synchrotron beamlines with extended spatial coherence and high intensity, equip end-stations for high-throughput lithography	Same as for nanopatterning. In addition: widespread dissemination of knowledge and collaboration between researchers and industrial developers	Develop resists with molecular resolution

Table 2.1.1: Nanostructuring of surfaces.

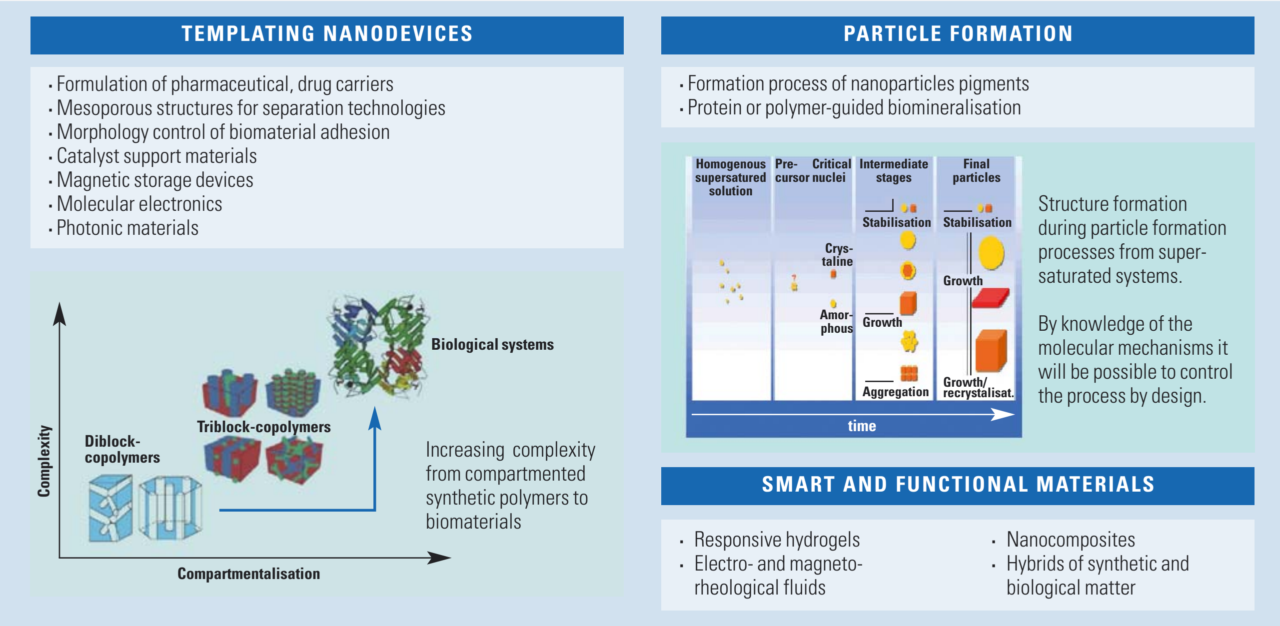


Fig. 2.1.3: A schematic of the importance of self-assembly in the context of nanomaterials.

- The detailed microscopic information on the composition and strain profiles within single nanostructures and on the occurrence of metastable structures during processing.
- Next-generation lithography will be based on so-called "extreme UV radiation" (EUV) with wavelengths of around 13 nm. Synchrotron radiation in this wavelength regime will become important for testing optical components necessary for EUV-lithography as well as for the development of the required photoresists. Surfaces of materials such as photoresists can be chemically modified by irradiation with soft x-rays.
- The use of coherent soft x-rays from synchrotron radiation facilities, which are used in order to create holographically, the necessary templates, must be better exploited in the future.
- Polymer grafting on the nanometre scale may provide an alternative to photoresist processes which are usually subtractive (parts of the resist are dissolved after exposure), and binary in terms of contrast. When polymer films (e.g. ETFE or FEP) are exposed to EUV synchrotron radiation, radicals are created near the surface of the polymer film which may serve as initiation centres for a subsequent graft-polymerisation process, yielding brush-like grafted polymer structures.

2.1.4. SELF-ASSEMBLY

Self-assembly of soft matter materials such as amphiphilic molecules, block-copolymers, surfactants, etc. into supramolecular structures offers an unprecedented variety of morphologies that can be used to create nanoscopic structures and functionalities. The control of this molecular self-organisation by means of chemical and physical stimuli is the key to the successful creation and control of structure on the nanometre and micrometre scale. The use of self-assembly ranges from the development of new formulas for pharmaceuticals and pigments to morphology control, to adhesion of biomaterials, to the development of molecular electronics, and to biomimetic crystallisation.

Future challenges

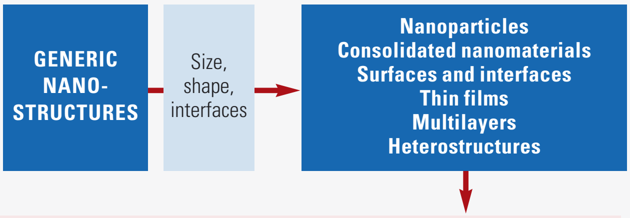
- To access the microscopic information on all levels of the self-assembled structures in a non-destructive way during all steps of the self-assembling process;
- To monitor the electronic processes within individual self-assembled structures in real-time;
- Development of a reliable database for self-assembly.

Future role of synchrotron radiation and neutron facilities

- Dedicated synchrotron radiation and neutron beamlines for developing self-assembly phase diagrammes;
- Special neutron diffraction beam lines (radiation damage-free !) for small and wide angle scattering to access the internal structure of the self-assembled nanostructures, of their size and of their spatial correlation in the liquid solvent.

2.2. NANOSTRUCTURES

The properties and functions of future nanomaterials will be intimately related to subtle aspects of their atomistic architecture. This includes the size and shape of the individual nano-"building blocks" (ranging from nanolayers to nanodots) and in particular their arrangement within the system (thin films, multilayers, lateral nanostructures). In most cases it is the interaction between these building blocks which determines the function. In turn, the understanding of phenomena at and across interfaces will become a key factor for the tailoring of nanomaterials, drugs, and nanodevices.



Future role of synchrotron radiation and neutrons
- Non-destructive 3-D information with sub-Ångstrom resolution;
- Non-destructive local information on electronic state;
- Diffraction and spectroscopy of nanostructures with sub-ppb impurity sensitivity;
- In-situ analysis of all relevant structural properties under relevant environmental and industrial conditions.

Fig. 2.2.1: Generic challenges for the characterisation of nanostructures.

2.2.1 FUNCTIONAL INTERFACES

The detailed understanding of the (chemical, electronic, magnetic) structure nature of solid-solid, solid-liquid, and solid-gas interfaces and of structural changes at these interfaces during the performance of the device is essential. It is apparent that this challenge calls for non-destructive in-situ technology for the characterisation of interfaces under environmentally and industrially relevant conditions.

Significant progress in the microscopic understanding of interfaces at relevant conditions is required for the rational design of nanomaterials which do not rely on rare, precious or toxic elements, or which can operate in environments such as the human body.

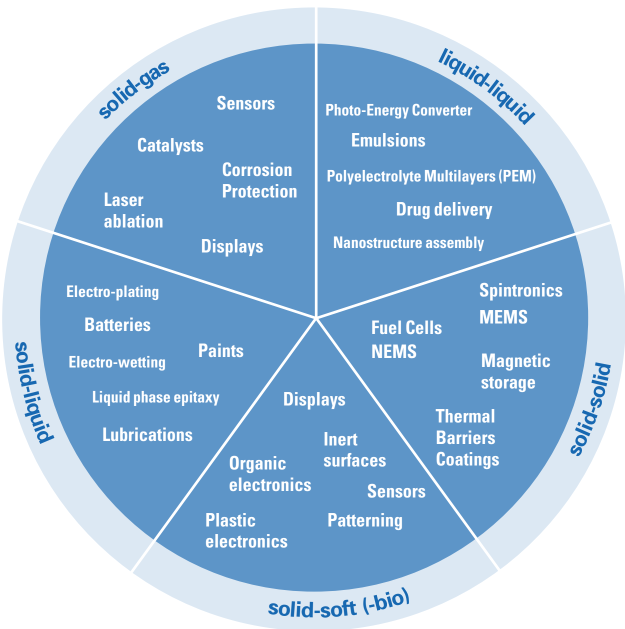


Fig. 2.2.2: The role of interfaces for future nanodevices.

A wide range of technologies is dependent on progress in surface and interface science (see Fig. 2.2.2). The technologies encompass both well-established areas with a large market volume such as catalysis, paint, batteries or corrosion, but also emerging technologies with significant economical potential such as fuel cells, plastic electronics and spintronics.

State of the art

Detailed information on the chemical, electronic and magnetic structure is available for single crystal surfaces under ultrahigh vacuum (UHV) conditions and for well-controlled exposure of adsorbates up to a full monolayer. The necessary analytical techniques are well-established and encompass STM/AFM techniques, surface x-ray diffraction, low-energy electron diffraction (LEED), AUGER spectroscopy, photoelectron-spectroscopy, x-ray surface standing waves. Dedicated synchrotron radiation beamlines for surface diffraction belong to the standard instrumentation at every synchrotron radiation facility world-wide.

Future needs

In the future the need for in-situ, non-destructive and real-time analytical access to all microscopy structural elements of (buried) interfaces and surfaces under realistic environmental and industrial conditions or even during the operation of a device will strongly increase. Since tunnelling spectroscopy methods are unable to access buried interfaces as well as surfaces which are in reaction chambers, the need for an analytical technology which can be used to determine surface and interface structures under all kinds of conditions will strongly increase as soon as the step from idealised conditions to real working conditions is performed.

Future role of synchrotron radiation and neutrons

Synchrotron radiation and neutron instrumentation will be increasingly necessary for the in-situ investigation of interfacial structures in gas-solid-, solid-solid-, solid-liquid-, and liquid-liquid interfaces. The challenge for the synchrotron radiation and neutron facilities is to provide the necessary beam quality and experimental support for the demands of the very large nanomaterials and nanotechnology community dealing with interface-controlled phenomena.

Solid-Gas Interfaces. The microscopic understanding of how nanomaterials behave and eventually deteriorate under environmental conditions and under various gas atmospheres, is important to be able to predict and control the stability and reliability of nanotechnological systems and structures. Controlling gas/solid interfaces plays a dominant role for key technologies such as catalysis, gas sensing and corrosion protection during thermal oxidation and synthesis of nanostructures from the gas phase.

The microscopic control of gas/solid interfaces under operational conditions is of utmost importance for the enhanced performance of catalysts involved in applications ranging from fuel cells and chemical production to electronic sensors for automotive and environmental

ROAD MAP SOLID-GAS INTERFACES

TECHNOLOGY	CATALYSIS & SENSORS	CORROSION PROTECTION	SYNTHESIS
STATE OF THE ART	Surface science approach: low p, T model catalysts in-situ study of single crystal surfaces	Ex-situ characterisation by TEM, in-situ by ellipsometry and weight change measurements	Ex-situ characterisation by TEM, and x-ray diffraction, trial and error to find growth recipes
FUTURE NEEDS	Design catalysts with chosen reactivity & selectivity, longer lifetime, cleaner production	Understanding & control of failure mechanisms, improve lifetime of protective layers, Develop self-repairing coatings	Preparation of well-defined atomically smooth Interfaces, homogeneous layers with chosen electronic & magnetic properties
ROLE OF INTERFACES	Reactivity zone, determines selectivity & reactivity	Protective layer adhesion, performance control	Reactive growth front, determines functionality
KEY BARRIERS	Pressure & materials gap between model systems and industrially relevant systems	Lack of understanding of failure mechanisms unclear role of interfaces	Lack of understanding of self-organised growth unknown interfacial structure during growth
RECOMMENDATIONS FOR SYNCHROTRON RADIATION AND NEUTRONS	In-situ characterisation of model nanosystems under industrially relevant conditions	In-situ time resolved (ns) corrosion studies at elevated temperatures, In-situ observation of interfacial structures and growth stresses	In-situ monitoring of growth processes on a atomic level, determination of interfacial structures,time-resolved experiments

Table 2.2.1: GENNESYS roadmap for solid-gas interfaces.

monitoring applications. Catalysts with a longer lifetime, larger turnover rates, and higher selectivity are needed. Thin films or nanoparticles with specific electric and magnetic properties that are controllable on an atomic level should be produced such that they are thermally stable and passive to oxidation.

These different technologies all imply processing conditions varying over a large gas pressure ranging across the bar regime and involving exposures to (corrosive) gases and temperatures up to 1500 K or even higher.

The key barriers for the development of new catalysts include:

- Lack of in-situ characterisation capabilities during operation;
- Lack of quantitative understanding of the influence of the material's morphology upon the gas reaction process;
- Unexplored role of dissolved gas atoms in subsurface regions of the material taking part in gas reactions;
- Unknown electronic structure and thermodynamic behaviour of nanosized particles and adsorbates;
- Unexplored nanomaterial/support interactions in the presence of gases.

Future needs

To be able to extract new, valuable knowledge from basic gas/solid interface studies for industrial applications, a non-destructive characterisation of model systems over length scales from metres to picometres, and timescales from hours to femtoseconds under technologically relevant operation or growth conditions is required.

Future role of synchrotron radiation and neutrons

- Structural and electronic characterisation of surfaces, interfaces, and nanoparticles with pm resolution in the presence of dense gas atmospheres under operation conditions (high p, T) using x-ray diffraction and absorption spectroscopy techniques and dedicated sample environments.
- Systematic investigation of the *kinetics* of gas solid/interface reactions using highly brilliant synchrotron radiation down to the

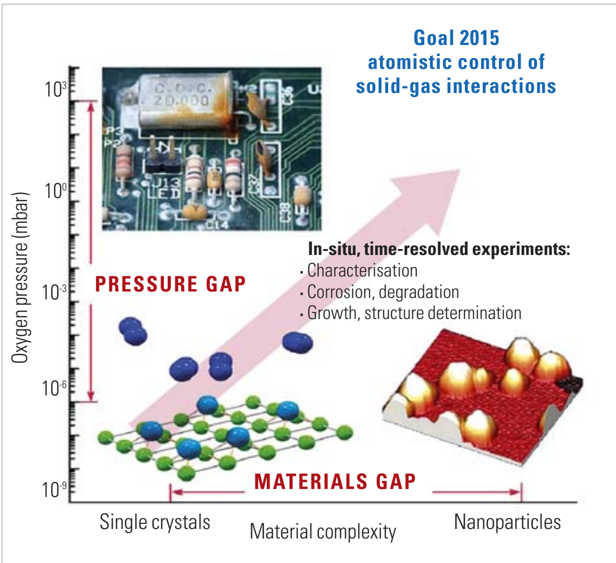


Fig. 2.2.3: Solid-gas interfaces: bridging the pressure gap and the materials gap.

ns timescale by a combination of fast detection chains and the exploitation of the specific time structure of the electron bunch.

- Information on the *transient states* during the initial interaction gas-surface interaction and their dependence on the energy and momentum of the gas molecule or particle which are the key to understand the microscopic details of oxidation, corrosion and catalytic processes. These transient states are elusive and require dedicated efforts combining pulsed, supersonic molecular gas sources synchronised with pulsed x-ray beams.
- Bridging the pressure gap and the materials gap in materials oxidation and corrosion: During the past 20 years, essentially the chemical and electronic structure of UHV prepared single crystal surfaces have been investigated as well as the structure of model adsorbates deposited under near-UHV conditions. In order to understand and control chemical reactions on real surfaces under real conditions, joint efforts are necessary combining different analytical technologies (x-rays, STM,...) with DFT calculations. Current European efforts already demonstrate the potential of this approach.

(a) Solid-liquid interfaces

The atomistic insight into solid-liquid interfaces plays a key role in many technologies, including energy conversion and storage (fuel cells and batteries), electrocatalysis and electrosynthesis, electrochemical & biosensors, corrosion protection, electrochemical refinement and purification, electrochemical nanostructuring and nanopatterning. Future progress in the field relies on the availability of in-situ techniques to probe structure, composition and dynamics of the interfacial region, in particular the uppermost layers of the solid phase in contact with the interfacial liquid layer.

Key barriers

- Lack of information on the structure of the interfacial region (chemical structure, charge distribution, adsorption, etc.).
- Insufficient understanding of the interface dynamics and charge transfer.
- Insufficient understanding of structure-composition-function in electrochemistry and electrocatalysis.

TECHNOLOGIES				
Electrocatalysis & electrosynthesis	**Energy conversion: Fuel cells & batteries**	**Electrochemical & bioelectrochemical sensors**	**Electrochemical phase formation & nanopattering**	**Corrosion protection**
ROLE OF INTERFACES				
Charge distribution; adsorption; electron/ion transfer; oxidation/reduction, confinement effects				
Activities & selectivities	Performance	Selectivity & performance	Composition & structure	Stability/degradation
STATE OF THE ART				
• Trial & error approach to materials design	• Insufficient performance • High costs • Insufficient long-term stability • Trial & error approach to materials design	• Insufficient selectivity • Trial & error approach to materials design	• Lack of structure control	• Material degradation
FUTURE NEEDS				
• Materials by design with desired electrocatalytic properties	• High performance devices	• High selectivity sensors	• Controlled nanopattering	• Understanding corrosion mechanisms • Novel protection strategies
KEY BARRIERS AND CHALLENGES				
• Insufficient understanding of interfacial structure and dynamics • Lack of understanding of structure, function relationships and confinement effects			• Insufficient understanding of phase formation	• Insufficient understanding of corrosion & protection mechanisms
RECOMMENDATIONS & GOALS				
Probing interfacial structure and dynamics in real-time and down to the atomic scale under operational conditions Real-time monitoring of charge transfer, adsorption, electrocatalysis, phase formation, segregation, restructuring, confinement effects High throughput analysis of promising functional materials In-situ real-time monitoring of long term stability, degradation and failure of functional materials				

Table 2.2.2: Future needs for electrified solid-liquid interfaces.

Future role of synchrotron radiation and neutrons

- Focused efforts have to be undertaken to exploit the in-situ characterisation potential of synchrotron radiation and neutrons to investigate electrified interfaces at different temperatures. This can be done during electrochemical processes accompanied by vigorous perturbations of the interfacial region, in particular for metal deposition/dissolution processes, inclusion and intercalation phenomena, and the proton motion in polymer matrices.
- Probing interfacial structure and dynamics *in real-time* and *down to the atomic scale*.
- Real-time monitoring of charge transfer, adsorption, electrocatalysis, and phase formation.
- Real-time monitoring of segregation, restructuring, confinement effects.
- High throughput analysis of promising functional materials.
- In-situ real-time monitoring of long-term stability, degradation and failure of functional materials.

Advancement in these fields will lead to the development of novel functional materials of superior quality for energy conversion and storage, electrocatalysis and electrosynthesis, electrochemical and biosensors, and corrosion protection.

SOLID-LIQUID INTERFACES IN CORROSION PROTECTION

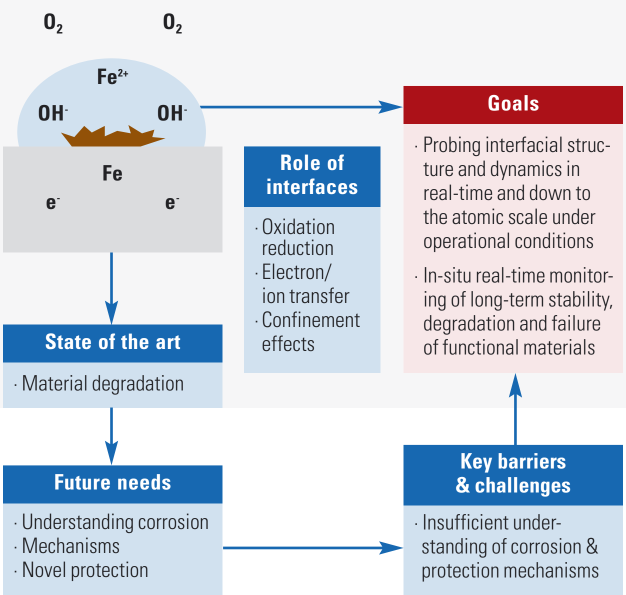


Fig. 2.2.4: Future challenge: microscopic control of corrosion.

Solid-liquid interfaces play a key role in the future development of nanofluidics and nanotribology which crucially depends on our knowledge about the microscopic processes at the liquid-wall interface. Most properties of confined fluids (spreading coefficient, adhesion force, capillary force, and viscosity) may in the future be controlled by the structural and chemical properties of the surrounding walls. Confinement on the nanometre scale strongly influences the flow of the fluid's particles or molecules as well as the fluid's freezing behaviour. Complex fluids such as colloids tend to crystallise more readily in confined geometries than in the bulk. Understanding such phenomena is relevant for the design of narrow flow channels, sieves, functionalised surfaces and wet labs on a chip.

The economic relevance of confined lubricating fluids is evidenced by the estimate that the annual losses due to friction and wear amount to ca 5% of the gross national product (GNP). A reduction of these losses by even a small amount results in substantial economical and

ROAD MAP SOLID-LIQUID INTERFACES

TECHNOLOGY	NANOFLUIDICS	NANOTRIBOLOGY
STATE OF THE ART	Lithographic fabrication of nm channels, demo of confinement effects, simulation of fluids in nano-scale pores	Measurement of frictional properties with SFA and AFM, deviations from 'laws' of friction found
FUTURE NEEDS	Control of fluid's properties through confinement, templated growth of e.g. protein crystals from solution	Control of friction at nanosized (lubricated) contacts, nearly frictionless contact superlubricity
ROLE OF INTERFACES	Nucleation site for crystallisation, confinement induced ordering phenomena, selective adhesion of (bio-)molecules	Boundary lubrication, confinement induced viscosity change in lubricant
KEY BARRIERS	Difficult access to interface, fabrication of ultranarrow channels	Lack of understanding of frictional forces and of stick slip phenomena, fabrication of reproducible nanocontacts interfaces
RECOMMENDATIONS	X-ray scattering from nanocavity arrays or single nanopores	Simultaneous determination of forces and of the lubricants' structural and dynamical properties using x-ray scattering and x-ray photon correlation spectroscopy

Table 2.2.3: Future challenges in nanofluidics and nanotribology.

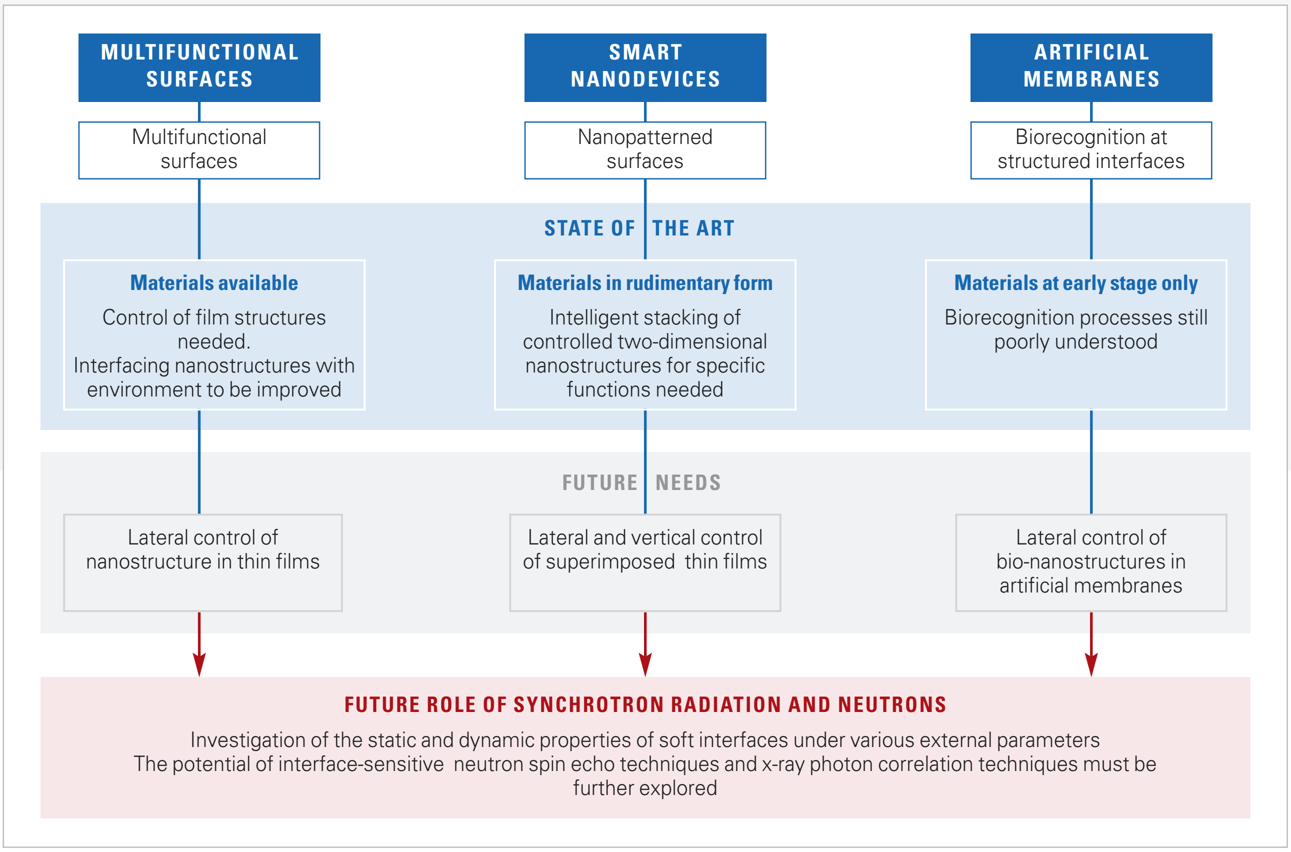


Table 2.2.4: Future challenges for soft interfaces.

ecological profits. Friction and wear will become a major issue in the operation of nanomachines, since they have large surface to volume ratios. The future vision is the fabrication of nearly frictionless contacts (superlubricity). It is now necessary to design an interdisciplinary research effort to explore the properties and behaviour of fluids at interfaces and in nanoconfinement.

(b) "Soft" interfaces

The structure of interfaces between inorganic and organic materials will play an important role in all future devices which exploit the properties of soft materials, i.e. polymers, organic molecules and biomolecules. The potential of soft matter lies in the enormous richness of properties which can be tailored by chemical modifications of the large molecular architectures. New applications based on soft materials range from organic electronics, chemical sensors to biocompatible films. Supramolecular materials built from highly regular nanostructures possess interesting visco-elastic or electric properties, and may respond sensitively to various external perturbations (sensors). The interface between the soft material and the substrate determines very often the performance and lifetime of such device. Furthermore, pattern formation by self-assembly, self-organisation or controlled dewetting can be exploited using tailored soft materials. Competing factors controlling the structure formation are chemical differences, conformational entropy, spatial constraints (molecular shape effects, chain stiffness) and external fields (electric, magnetic, hydrodynamic flow, structured surfaces).

Lateral and vertical control of nanostructured surfaces is necessary to obtain smart nanodevices. Such devices could be based upon structures of self-assembling polymers forming pores of controlled shapes under physico-chemical control. An example is intelligent control by mechano-chemical valves.

A complete new area comes up with the introduction of bio-aspects in nanostructures. Learning from nature potentially allows a versatility and subtle handling of complex hierarchies that is unprecedented in terms of specificity and precision. This is expected to bring new developments regarding biological functions in material surfaces and interface, sensing, biomimetic functionality, biohybrid materials. Such developments will also facilitate new routes in material and tissue engineering.

Future challenges and open questions

- How can nanostructured polymeric surface patterns be employed as templates for the fabrication of novel materials and functional devices?

- How do the physical properties of such nanostructured patterns depend on the structure of the interface?
- Which structural features (aperiodic structures, directional interactions) need to be improved or optimised for devices?

Future role of synchrotron radiation and neutrons

- Detailed microscopic information on the structure of thin films made from soft materials is essential for the future goal of tailored fabrication of devices. Neutrons will play an increasingly important role, since they can penetrate material, do not create radiation damage and can be rendered sensitive to interfaces.
- It must be explored if the unambiguous determination of the complex structures associated with soft matter and the associated interfaces can be better done by x/n contrast diffraction experiments. In order to explore irreversible changes at soft interfaces the need for a European beamline which provides glancing angle and small angle x-ray and neutron scattering should be analysed by the facilities which are in close contact with the soft matter community.
- The dynamic behaviour of soft interfaces, i.e. capillary motion, needs to be analysed on a microscopic level, in particular its dependence on the interfacial interactions. For this, x-ray photon correlation spectroscopy and neutron spin echo spectroscopy instrumentation should be optimised to address this important phenomenon.

(c) Solid-solid interfaces

Solid-solid interfaces are the omnipresent structures in many nanodevices. In all thin film and multilayer devices the structure and processes at the solid-solid interface decide if the device works at specification. In fact, many degradation and failure mechanisms in thin film and multilayer devices start at the internal interfaces. The key structural features are the atomistic chemical, electronic and magnetic structure of the interface, including details on the interfacial interactions, interfacial roughness, strain and composition gradients. A current and future focus in fundamental research is on the understanding and control of the magnetic interaction across interfaces (GMR devices) and on the electronic transport across interfaces, in particular, electron tunnelling at metal-insulator interfaces and spin-dependent electronic transport at ferromagnet-semiconductor interfaces.

In nanomechanical devices, friction and lubrication at sliding solid-solid interfaces will become a key parameter which controls the performance and lifetime. Although friction has been studied for many years, it is not possible today to predict the friction coefficient for any given pair of materials (as metal-ceramic couples) under specified conditions. Among the unknown parameters which affect the coefficient are the role of the oxide layer, the roughness of the sliding surfaces, and the structural changes during sliding (including melting at higher speed).

State of the art

By their very nature, solid-solid interfaces are buried and thus very difficult to access experimentally. All routine surface analytical tools working with electrons as probes (electron diffraction, photoelectron spectroscopy), or use tips (STM and AFM) cannot be applied. In the last decades x-ray and neutron reflectometry and off-specular diffraction have been developed to a high level of sophistication and maturity. They now provide laterally averaged information on the structural profile across the solid-solid-interface. Recently, a new transmission-reflection scheme has been devised which is able to access deeply buried interfaces with high-energy x-ray microbeams. Friction at solid-solid interfaces has been studied by sliding AFM tips, thereby emulating the situation that at most solid-solid interfaces of technological relevance, contact occurs at numerous asperities.

Future needs

- Since solid-solid interfaces already exist in operational devices (as in GMR read heads), the demand for standardised information on all structural parameters of solid-solid interfaces will increase very strongly in the near future, as for standardised measurements of the interfacial roughness.
- The structural changes at solid-solid interfaces during performance have to be understood with highest reliability and precision (interdiffusion, residual and thermal strain).
- The magnetic interaction in multilayered structure, in particular the nature of the exchange bias has to be explored in a systematic way.
- A microscopic insight into friction and lubrication at solid-solid interfaces is urgently required. The goal is to relate friction and wear to the atomistic dissipative reactions at the interface.

Future challenges for synchrotron radiation and neutron facilities

- Nanometrology stations using standardised instrumentation for characterising solid-solid interfaces need to be installed at synchrotron radiation and neutron facilities.
- Synchrotron radiation instrumentation for the resolution-free measurement of interfacial roughness using fully coherent x-ray beams has to be developed. These efforts need to be accompanied by the associated theoretical efforts to reconstruct the full 2-D-roughness from the recorded speckle intensity distribution.
- Systematic neutron studies of magnetic interactions and spin structures in complex multilayers.
- Real-time diffraction and spectroscopy studies for the in-situ study of sliding friction between two solid interfaces using free-electron x-ray laser radiation.

2.2.2. THIN FILMS AND MULTILAYERS

Thin film and multilayer-based technologies have experienced expotential growth in the past 15 years. Functional thin films are used today in many systems for tailored electronic, magnetic, optical, chemical and thermal properties. The current state of microelectronics and optics is unthinkable without the enormous advancement in thin film technology. Thin films serve also as chemical sensors, chemical protection layers, thermal barriers, and for wear protection. It is expected that in the next 10 years, most future key technologies will be based on thin film and multilayer devices.

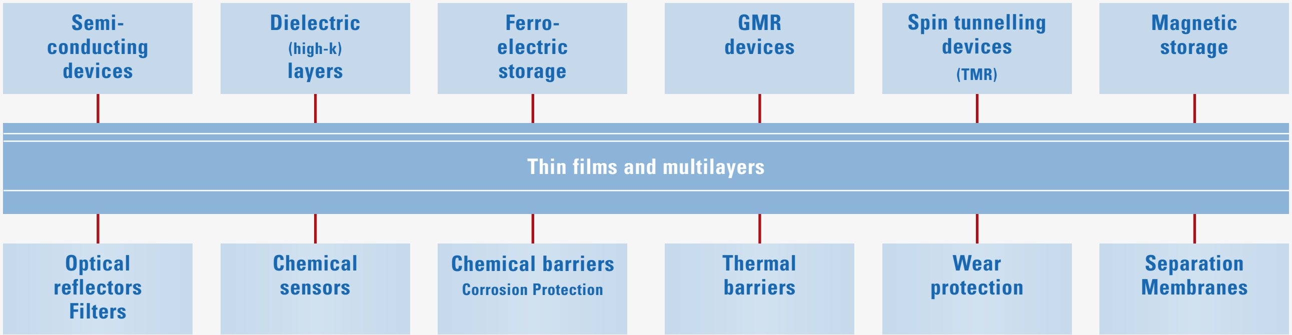


Fig. 2.2.5: Thin films and multilayers in current and future technologies.

In thin films and multilayers, one length scale (thickness of the film and of the individual layers, respectively) is under external control. The precise control of this nanolength with atomic resolution renders such systems a key area for nanotechnology. By a clever combination of materials, new phenomena which do not exist in nature can be evoked by the one-dimensional non-confinement and by the crosstalk between the adjacent layers ("proximity effects"). Illustrious examples of this are the Quantum Hall Effect discovered in semiconductor multilayers, used today as a quantum standard for the electrical resistivity or the Giant Magneto-Resistance (GMR) effect discovered in Co-Cu-multilayers used today as a new reading head in hard disc drives. Future research will increasingly focus to access and control the nanometre size and onto so-called hybrid systems which bring rather different materials classes in a nanocontact.

State of the art

Thin films and multilayers are routinely investigated today using well-established synchrotron radiation and neutron techniques which provide atomistic information. The most popular tools are reflectivity studies and many derivatives of glancing angle diffraction as well as x-ray standing waves which provide depth resolved information. In these routine investigations the x-ray and neutron beam averages the inplane structural properties of the thin film and multilayer structure. More sophisticated analytical techniques have emerged in the past that exploit x-ray imaging and x-ray microscopy techniques exhibiting lateral resolution down to 30 nm.

Future challenges

Many future analytical challenges in thin films and multilayers are clearly material-dependent and will be addressed separately in Chapter 3. However, there are also several generic problems associated with the structure of thin films and multilayers requiring a dedicated use of synchrotron radiation and neutrons in order to understand and control these phenomena:

- The performance of future thin films or multilayers is and will – even more in the future – be determined and often controlled by the structure of and the phenomena at its solid-solid interfaces; thus, all the key barriers and future research needs summarised in section 2.2.1, also hold here. In fact, the standardised characterisation of surface and interfacial roughness will become a key need in many of the thin film technologies, since this structural feature will start to dominate as the thickness of the films and layers decreases to the nanosize.
- In the future, complex (multicomponent) thin films and multilayers will emerge that have a heterogeneous structure and different properties parallel and normal to the growth direction. A key challenge

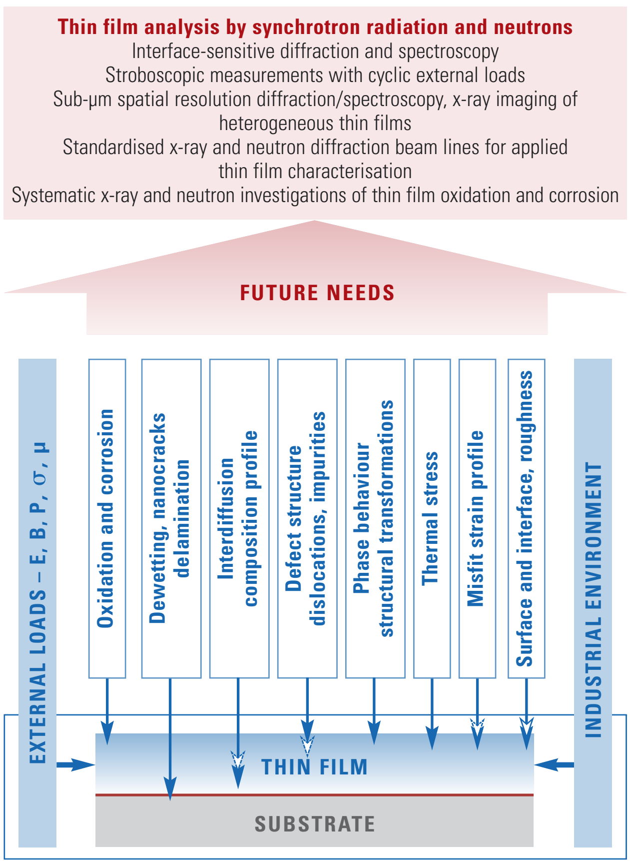


Fig. 2.2.6: Challenges for synchrotron radiation and neutrons in the structural characterisation of thin films.

is thus to have destruction-free analytical tools available providing a fully three-dimensional (non-averaged) image on the atomic scale.

- The performance and lifetime of thin films is determined by misfit strain and thermal strain. It is necessary to develop an analytical technology, able to monitor misfit strains with a high level of sensitivity and in a quantitative fashion.
- Subtle structural changes during operation (strain, dewetting, roughening, interdiffusion) are of key importance for the microscopic control of the performance and for monitoring the degradation of the device.

Future research needs and the role of synchrotron radiation and neutrons

- Thin film and multilayer technologies urgently require nondestructive testing beamlines at synchrotron radiation and neutron facilities for a full quantitative characterisation of all structural details, incl. strain gradients, composition gradients, and interfacial roughness parameters. These beamlines must in particular be accessible to industrial partners, thus, require easy access, stable operating conditions, standardised structural information, and confidentiality in data handling.
- Synchrotron radiation and neutron facilities have to design analytical tools which deliver non-averaged information on heterogeneous thin film and multilayer structures. It is of utmost importance to explore the limits for nanobeam technology and the conversion of imaging and microscopy techniques into a routine analytical technology for quantitative analysis.
- Synchrotron radiation facilities and future free-electron laser facilities must explore the analytical potential of fully coherent diffraction for the investigation of thin film and multilayers. Of particular importance are time-resolved monitors for the development of nanocracks in thin film structures.
- Thin film and multilayer technologies urgently require nondestructive testing beamlines at synchrotron radiation and neutron facilities for long-term studies of degradation and failure analysis on a microscopic level.
- Systematic synchrotron radiation and neutron in-situ measurement of losses in thin films and multilayers in order to identify – at several length scales – the mechanisms for degradation and failure in high power applications, as in actuation technology (piezoactuators) and in control applications are urgently required.
- In-situ x-ray and neutron diffraction studies of interdiffusion, roughening, strain development in thin film and multilayer materials and devices under realistic conditions will be urgently needed for performance and quality control. In some cases this in-situ monitoring must be done with a lateral resolution of less than a µm.
- The semi-continuous synthesis process of many coatings are controlled by a rather complex interaction of the several control parametres that are only very roughly understood. Thus, there is an urgent need for a quantitative coating process control and for:
  - testing methods, in particular for the build-up of internal stress;
  - the calibration of monitoring methods for structural parameters (incl. the internal stress) under factory floor conditions;
- The dewetting of organic and polymer thin films must be studied systematically using neutrons (no radiation damage) in a time-resolved mode.
- Fundamental research using neutron reflectometry and magnetic x-ray diffraction must be continued to clarify magnetic coupling mechanism in magnetic multilayers, including the origin of the exchange bias.

2.2.3. NANODOTS AND NANOWIRES

Novel materials architectures based on nanodots and nanowires exploiting new (ultimately quantum) properties belong without a doubt to the supreme discipline in current and future nanomaterials research. Since the invention of the transistor, the semiconductor industry has been one of the major drivers for this continuous miniaturisation of materials structures (as described by Moore's law). This is moving now beyond the micrometre into the nanometre regime. The goal is the design of nanostructures with new properties for future technologies, in particular for the information and energy sector. Data storage capacities could reach the Terabyte/in^2, but nanodots and -wires carry the potential to evoke new phenomena in almost all sectors of materials functions ranging from mechanical to medical properties.

State of the art

During the past 20 years, STM and AFM have proven to be an ideal and indispensable tool for characterising and manipulating single nanostructures. With the use of magnetic tips even the characterisation of the magnetic structures of individual nanodots is possible today. Undoubtedly, many future analytical challenges will further be met by exploiting the enormous potential of these lab-based scanning tunnelling probes. Synchrotron radiation applications have been used to explore the internal composition and the strain state of the semiconductor nanodots. These x-ray studies have provided structural information on the "average nanodot". Recent attempts have been made using fully coherent beams to access the information from individual nanodots.

Future challenges

The future need:

- To access the microscopic information on subtle structural features within individual nanostructures, such as composition and strain gradients;
- To observe the structural changes of single nanodots under realistic ambient conditions (oxidation, corrosion, interdiffusion);
- To precisely characterise embedded nanodots in a non-destructive way;
- To characterise the processing and the structure of functional nano-units in three-dimensional arrays and, ultimately,
- To monitor structural and electronic processes within individual nanostructures during device operation in real-time in a non-destructive and standardised way will steadily increase with the sophistication of these nanostructures and with the attempt to con-

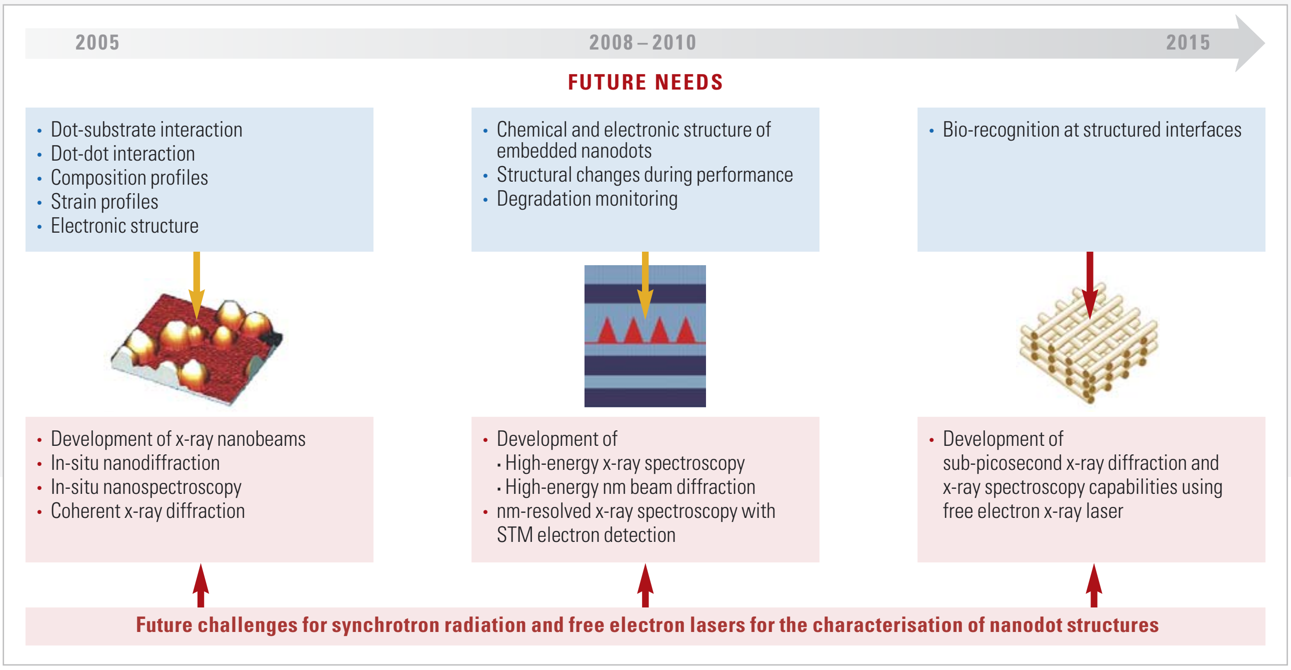


Fig. 2.2.7: Challenges for synchrotron radiation in the structural characterisation of nanostructures of thin films.

vert these structures into useful technologies, e.g. for nanolight sources (IR), enhanced optoelectronic devices, nanostructural spintronics devices or high speed switching devices.

Future role of synchrotron radiation and neutrons

- These future analytical needs produce very serious challenges to the roadmap of the large-scale facilities, particularly for the synchrotron radiation and Free-electron laser facilities which have to embark on the development of the necessary analytical concepts which are able to overcome these barriers.

- It is of key importance that all experimental concepts produce nano-x-ray beams are fully exploited in order to implement within the next 5 to 10 years all the analytical capabilities necessary to access individual nanounits under rather different conditions.These analytical concepts should allow for the extraction of relevant structural, electronic and magnetic properties in a standardised, non-destructive way that can display a high level of accuracy.

- The potential of x-ray imaging and microscopy must be explored systematically for the in-situ investigation of nanodot and nanowire structures.

- If such a non-destructive nanocharacterisation technology has been rendered reliable at current and future x-ray facilities, several dedicated beamlines for the standardised measurements of the function, performance and failure of three-dimensional nanostructure arrays should be designed and coordinated in a European network for the rapid access to the research laboratories from industry.

2.3. NANOMATERIALS PHENOMENA

Nanomaterials are the generic materials architectures for evoking new ("enabling") phenomena. The expectation is that unexplored new nanophenomena will emerge from three generic structural elements:

- The scale size of nanounits is coupled to an intrinsic length scale. A prime task for the future is the systematic investigation of the critical length scales that are associated with collective phenomena

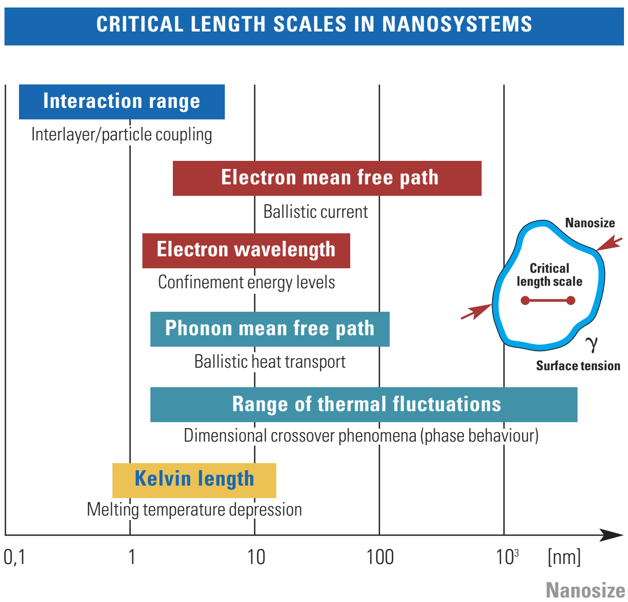


Fig. 2.3.1: Comparison of critical length scales and the size of the nanomaterials.

within the nanostructures. As a rule of thumb, new phenomena should emerge whenever the system size falls short of the intrinsic length associated with a collective phenomenon.

- The large surface area of nanounits creates a huge amount of surface structures and surface states producing properties different from the bulk, and allow an exponentially enhanced interaction of the material with the environment.

- The nanoscale arrangement between the nano-units in tailored 1-, 2- and 3-dimensional architectures allows a tailored interaction and a tailored materials-, charge-, spin- and energy-exchange between different materials ("proximity").

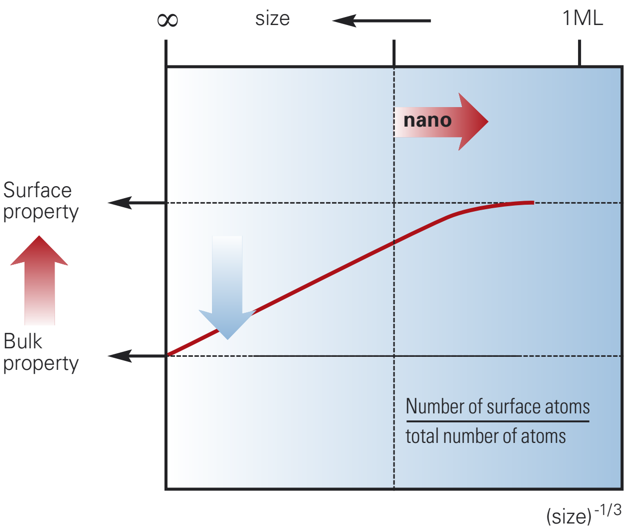


Fig. 2.3.2: Appearance of surface properties versus size.

State of the art

Nanophenomena are investigated today in many laboratories (mainly universities) by many different experimental techniques within local research programmes. At synchrotron radiation and neutron facilities these investigations are a natural part of the routine user programme. Unfortunately there is no coordination of efforts.

Future challenges

Scaling laws and size-dependent phenomena should be established experimentally to be used as a basis for theoretical models. Here, a clever interplay of different analytical tools ranging from x-ray and neutron diffraction to imaging, tomography, and microscopy appears as the most promising strategy. This is achieved by improving and coordinating the access to costly analytical technology to the European researchers.

Nanomaterials are by nature high-speed materials and thus promising candidates for the storage of information and for nanomechanics. The relevant relaxation times and their limits are insufficiently explored. This holds in particular for magnetic, electric, and multiferroic materials. The experimentally accessible time scale by in-situ x-ray and neutron analysis ranges from hours down to the sub-picosecond regime. The new x-ray lasers being developed in Europe as well as dedicated spin-echo techniques to be implemented in future neutron spallation sources should play a key role in this most promising research area.

The investigation of these "enabling nanophenomena" is very clearly a very promising future discovery field best explored by small creative research groups which should work in a healthy competitive funding environment allowing flexibility and mobility for young researchers.

The exploration of nanomaterials properties for new applications will face many key barriers. It is thus equally important to investigate in detail those nanophenomena which pose limits or limitations to the exploitation of nanomaterials in new technologies. Here, one could think of interdiffusion, corrosion, or strain-induced degradation of nanostructures ("disabling phenomena"). Many of these disabling phenomena require systematic and long-term studies in order to find alternative ways to overcome the problem.

Recommendations for future role of synchrotron radiation and neutron facilities

All x-ray and neutron technologies (diffraction, spectroscopy, tomography, imaging, microscopy) must be explored for the systematic characterisation of nanomaterials phenomena exploiting their unique properties. It must be further analysed, how converging methods between x-rays and neutrons and other analytical techniques have to be conceived in order to fully understand nanophenomena in complex materials systems.

Of particular importance are:

- Systematic studies using x-ray and neutron techniques to set up a reliable database for nanoparticle-substrate interactions and for adhesion and wetting phenomena
- The availability of dedicated x-ray and neutron beamlines in combination with other analytical complementary techniques for the combinatorial search of new phenomena in nanomaterials
- The development of the necessary x-ray and neutron technology for time-resolved structural and electronic investigations
- The availability of dedicated x-ray and neutron beam lines for systematic studies of limiting phenomena which lead to materials failure, in particular nanofatigue, segregation, interdiffusion, electromigration, dewetting, microscopic precursors of delamination, structural transformations, and interfacial roughening under various (realistic) conditions
- The in-situ x-ray and neutron studies of corrosion and friction processes under relevant conditions.

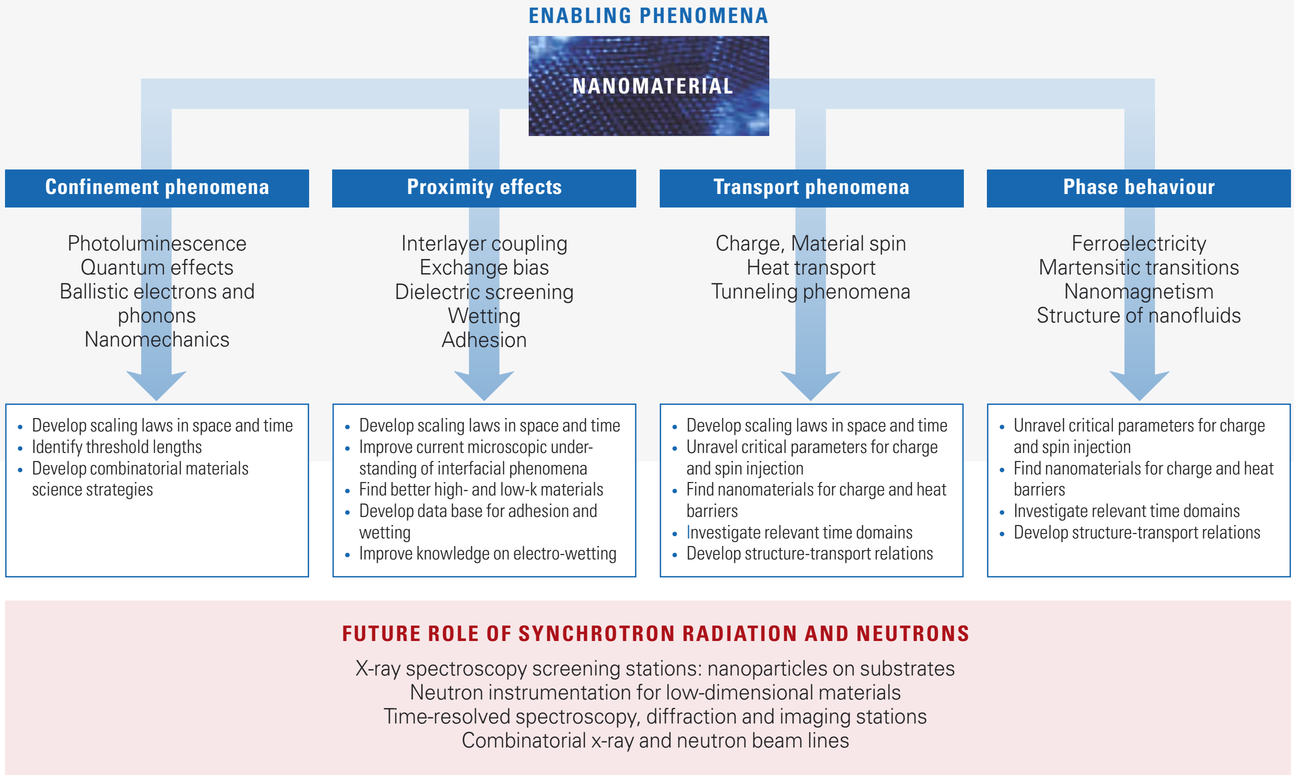


Fig. 2.3.3: Enabling phenomena.

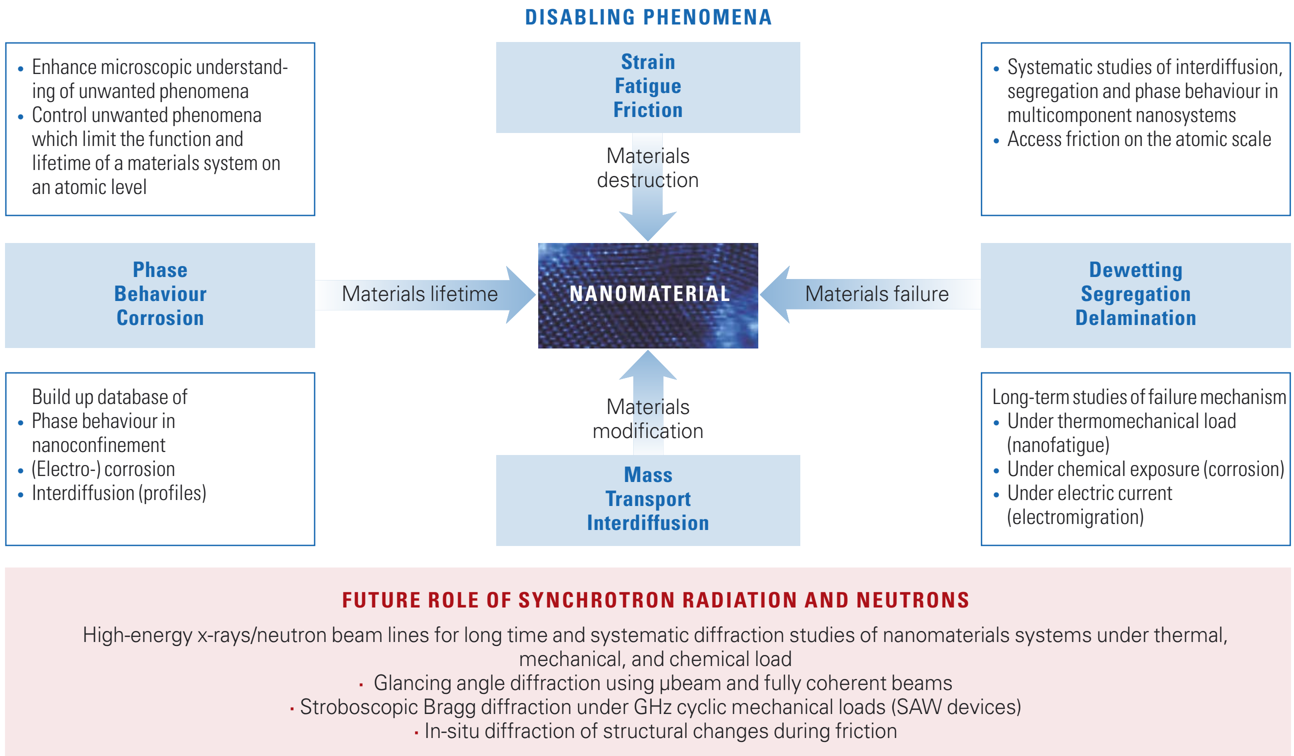


Fig. 2.3.4: Disabling phenomena.

2.4. NANOMATERIALS FUNCTIONS

The prime task of nanomaterials science is to unravel new materials phenomena, to exploit them for new materials functions and optimise them for improved or new applications. Nanomaterials functions with high innovation potential encompass:

- **Improved mechanical functions**
  lighter materials with higher strength, flaw-resistant hierarchical materials, NEMS, nanolubrication, nanofluidics,
- **New electronic functions**
  enhanced high-k and low-k properties, ferro- and piezoelectricity, tunable dielectrics, ballistic electronic transport,
- **New magnetic functions**
  nanomagnetism, ferrofluids, magnetic switching, spin-dependent transport,
- **Enhanced thermal functions**
  nano-invars, thermal barrier coatings, ballistic heat transport
- **Improved chemical functions**
  catalytic properties of nanoparticles, photocatalysis, corrosion protection,
- **Novel optical function**
  photoluminescence, photonic devices, highly reflecting, non-reflecting and selectively reflecting surfaces,
- **Biological functions**
  biocompatible surfaces, bioactive surfaces, drug carriers.

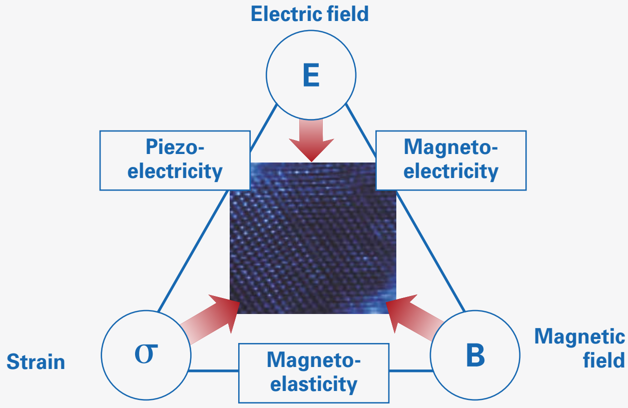


Fig. 2.4.1: Smart nanomaterials with multiferroic functions.

Future challenges

Future holy grails in the search for new functions are materials with exhibit:

- *Flaw-insensitivity* by hierarchical structures which do not allow crack propagation and heal nanocracks;
- *Complex adaptive (emergent) behaviour;*
- *Multiferroic functions* (piezo-piezoelectricity, magneto-electricity and magneto-elasticity).

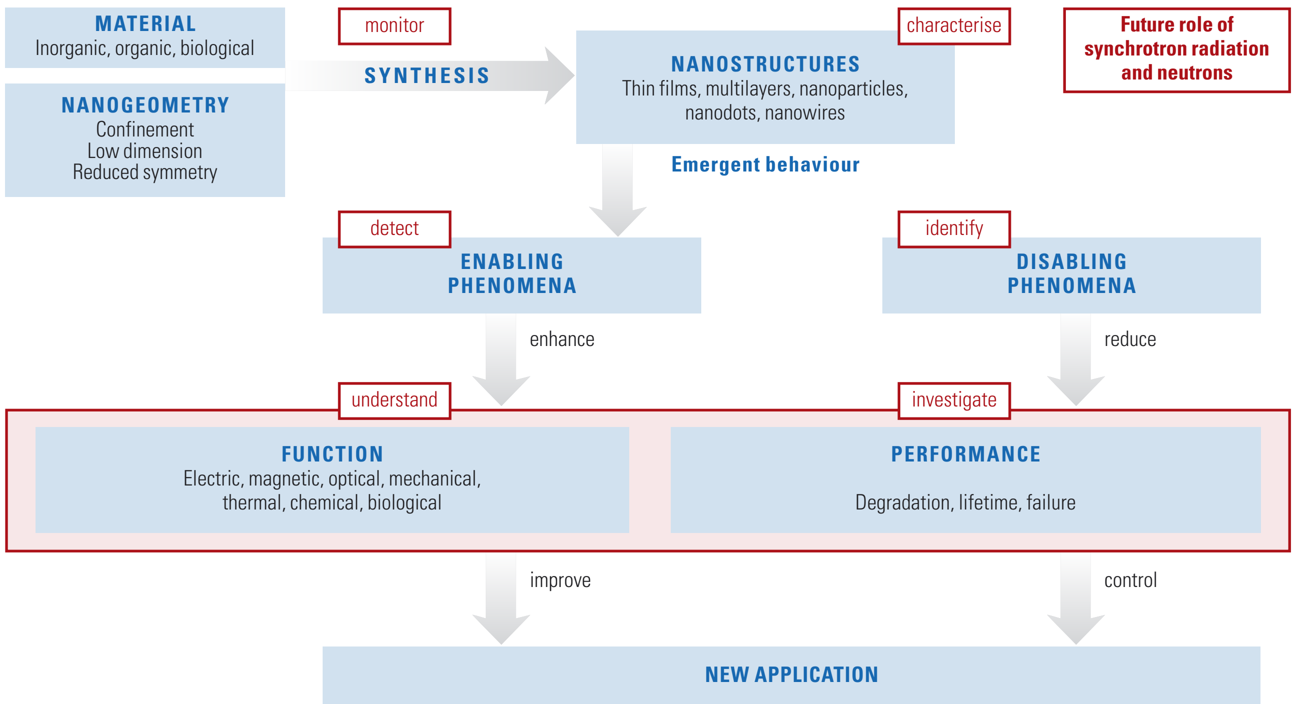


Fig. 2.4.2: The strategy to improve nanomaterials functions and performance and the role of synchrotron radiation and neutron facilities.

This transformation of a new phenomenon into a useful new function requires that the useful (enabling) phenomenon is enhanced and simultaneously the limiting phenomena are controlled and reduced to allow optimum performance. This function-design strategy requires microscopy insight into all details of the material at hand at each step of the design.

Future role of synchrotron radiation and neutrons

In this rather complex field of function design, synchrotron radiation, and neutrons will play a key role, since they allow to access the relevant microscopic information in a versatile way and under almost all environmental conditions.

The future tasks of synchrotron radiation and neutrons for enhancing nanomaterials functions and optimising the performance are as follows:

- Dedicated synchrotron radiation and neutron diffraction and spectroscopy beam lines integrating complementary analytical technology in order to establish the microscopic relation between the chemical, magnetic, and electronic structure of the material with the desired functions;
- Dedicated synchrotron radiation and neutron instrumentation to study the dynamic structural and electronic response of nanomaterials upon external stimuli (electric and magnetic fields, mechanical stress);
- High throughput synchrotron radiation and neutron beamlines for combinatorial investigation of structure-function relations;
- Dedicated synchrotron radiation and neutron instrumentation for performance studies of functional materials under different environmental conditions.

2.5. NANOMATERIALS MODELLING

In this section, we aim to identify challenges and opportunities for theory, modelling, and simulation in the research, development and tailoring of nanomaterials and in directing and optimising experiments using synchrotron radiation and neutrons.

2.5.1. MODELLING AND SIMULATION IN NANOSCALE MATERIALS SCIENCE AND NANOTECHNOLOGY

New capabilities in theory, modelling and simulation

During the last decades, density functional algorithms, quantum Monte Carlo techniques, ab-initio molecular dynamics, advances in mesoscale methods for soft matter, and fast-multipole and multigrid algorithms have been developed and refined. In parallel, advances in computing hardware have increased the available computing power by four orders of magnitude. The combination of new theoretical methods, together with the advanced experimental techniques and the increased computing power, has made it possible to simulate nanosystems with millions of degrees of freedom.

Industry will not risk large-scale manufacturing of a product or component unless it can understand the nanomaterial to be manufactured, and can predict and control the process to make products within well-defined tolerance limits. For macroscopic systems – such as the products made daily by the chemical, materials, and pharmaceutical industries – that knowledge is often empirical, founded on an experimental characterisation over the range of state conditions encountered in a manufacturing process. To attempt to understand nanoscale systems and to control the processes to produce them based solely on experimental characterisation is out of the question. Therefore, qualitatively new theories are needed.

Promise of theory, modelling, and simulation

The application of new and most advanced experimental tools to nanomaterials systems demands an urgent need for a quantitative understanding and description of the structure and dynamics of matter at the nano- and femtoscale, respectively. The absence of new tools and quantitative models which describe newly observed phenomena, direct the design and synthesis, and interact with the macroscopic world, would increasingly miss important scientific opportunities for discoveries in nanomaterials science. Moreover, this absence would seriously inhibit wide-spread applications in different fields of nanotechnology ranging from molecular electronics to biomolecular materials.

Nanosized systems modelling and electronic structure calculations

Electronic structure calculations of nanosystems are considered as a scattering problem, where centres of scattering are atoms of clusters. The coherent potential approximation (CPA) as an effective-medium-

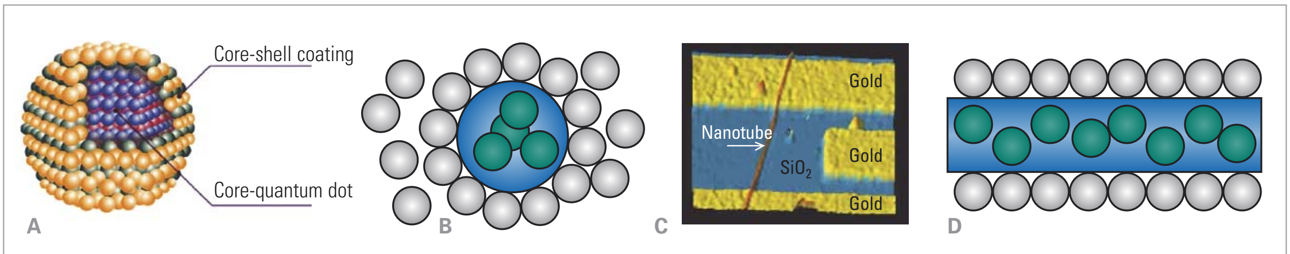


Fig. 2.5.1: Models of nanosystems: a) quantum dot realistic model; b) quantum dot cluster model; c) quantum wire with in integrated scheme; d) quantum wire cluster model.

approximation (EMA) variety yields good results in modelling. The cluster models of quantum dots and nanowires are presented in Fig. 2.5.1. The modelling starts with realistic analytical potentials (as scattering centres) construction for atomic clusters on the basement of special analytical procedure, taking into account interatomic Coulomb interactions, exchange, and correlation to create the model of electronic charge density.

The next step is the calculation of scattering properties of atoms and atomic clusters of modelled configuration. Cluster formations are placed in effective medium potential (usually, the coherent potential approximation-CPA is used). This allows to calculate the dispersion law E-k, electronic density of states, evaluate total energies and elastic constants, and estimate the conductivities. The multiple scattering problems are stated for radial (in cases of quantum dots) and axial (in cases of nanowires and nanotubes) symmetry approaches. This means the particular adequate to scattering problems symmetry Schroedinger equation splitting and scattering waves character (spherical or cylindrical).

Future tasks and challenges

The modelling of nanomaterials and nanodevices will play an eminent role within the GENNESYS project. The following challenges have been identified:

- Modelling transport mechanisms at the nanoscale: electron transport (molecular electronics, nanotubes); spin transport (spintronics-based-devices); molecular transport (chemical- and biological sensors, molecular membranes, and nanofluids);
- Devising theoretical and simulation approaches to study interfaces, which dominate (complex and heterogeneous in shape and substance) nanoscale systems;
- Bridging electronic through macroscopic length and timescales, so phenomena captured in atomistic simulations can be modelled at the nanoscale and beyond;
- Simulating complex nanostructures involving many molecular and atomic species: "soft" biologically or organically-based structures and "hard" in-organic ones as well as (soft/hard) interfaces between hard and soft matter;
- Simulating self-assembly and directed self-assembly, the direct key to large-scale production of novel structures;
- Modelling optical properties of nanoscale structures and to model nanoscale opto-electronic devices;
- Developing self-validating and bench-marking methodologies for modelling and simulation;
- Devising theoretical and simulation approaches to quantum coherence, deco-herence, and spintronics.

The development of future nanomaterials involves multiple length- and timescales as well as the combination of types of materials and molecules that have been traditionally studied in separate subdisciplines. For theory, modelling, and simulation, this means that different methods that were developed in separate contexts will have to be combined and new ones invented. While traditional materials modelling could often address electronic properties and chemical bonding characteristics in very simple geometries and with periodic boundary conditions, this is not possible on the nanoscale. Many opportunities with nanoscale functional materials lie in precisely the fact that function and size, shape or stress state are intimately connected. Modelling and simulation must therefore always be dealt with as a coupled problem where inhomogeneous stresses and complicated boundary conditions are inherited from larger scales, while chemical accuracy and electronic functionality have to be computed. This requires the formation of alliances and teams of nanomaterials scientists, experimentalists, theorists, applied mathematicians, and computer scientists.

2.5.2. MODELLING STRATEGY FOR SYNCHROTRON RADIATION AND NEUTRON EXPERIMENTS

A new class of computational tools

In addition to the development of new multi-discipline/multi-scale materials modelling methodologies, an optimal modelling strategy must be initiated for guiding synchrotron and neutron based experiments in the development and tailoring of functional nanomaterials. By virtue of their complex structure, nanomaterials offer interesting challenges to both simulation and experiment:

- Synchrotron and neutron facilities are faced with the challenge of developing novel techniques to interrogate smaller length- and shorter timescales.
- Traditional analysis procedures of experimental data, which often assume particular degrees of homogeneity and simplified statistics, are also faced with validity and developmental issues.
- Simulation is faced with the challenge of modelling larger, more realistic structures for longer periods of time. More importantly, it is expected to yield quantitative results that have an experimental context.
- Simulation is faced with the difficulty of achieving electronic information or chemical accuracy of the bonding characteristics while dealing with non-periodic boundary conditions or inhomogeneous stresses.

Convergence between experiment and simulation in both time and space therefore constitutes the central strategy of the present approach which, at its heart, relies on a new class of computational tools that simulate experiment. It is through such tools that atomistic simulation can:

- Gain a quantitative experimental context;
- Aid in the interpretation of experiment and associated analysis procedures;
- Guide the development of new experiments.

The flow of information is therefore bi-directional, in which new and emerging experimental techniques are employed with simulations on increasingly powerful computers leading to the desired convergence between simulation and experiment and the development of new and novel functional nanomaterials.

Simulating synchrotron and neutron experiments

At the forefront of such an approach is the development of computational tools that simulate x-ray and neutron experiments using atomic scale resolution data generated from simulation as input. Traditional experimental techniques that can be simulated are:

- Monochromatic diffraction and small angle scattering;
- White beam Laue microdiffraction;
- Inelastic scattering (triple axis and time-of-flight measurements).

The simulation of such experiments will:

- Allow the "experimental" characterisation of simulated microstructure providing for the development of more realistic atomic scale resolution configurations involving i.e. grain boundary networks, extended dislocation configurations, and more general defect structures such as interstitial and vacancy clusters;
- Aid in the interpretation of real experimental data, validate existing theoretical experimental analysis procedures, and give insight into the statistically meaningful quantities that experiment probes;
- Help in the identification of component processes, which through their number and strong interaction, lead to emergent processes;
- Allow for modelling of the experiments to guide experimentalists to the best use of their techniques;
- Lead to direct structure determination from experiment through (restricted) inverse modelling.

The simulation will lead to an improvement of experimental set-ups with respect: i) to their sensitivity; and ii) to the key structural and dynamic properties of the materials:

- Through their repetitive measurements, "pump and probe" synchrotron beam lines gain sufficient data to probe statistically significant ensembles at the sub-millisecond time scale;
- Nanodiffraction beam lines offer sub-micron spatial resolution;
- Femtosecond pulsed x-ray techniques also offer unprecedented time resolution for the probing of fast atomic scale processes.

This way, simulation and experiment might begin to converge. It also offers a path to overcome, or at least minimise, the length and timescale restrictions of atomistic modelling. The connectivity of this approach is schematically outlined in the diagramme shown in Fig. 2.5.2 and Fig. 2.5.3.

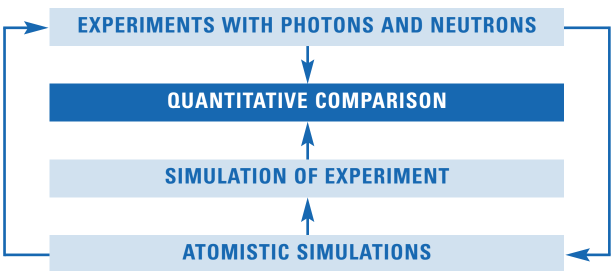


Fig. 2.5.2: Diagramme presenting the interaction between experiments and simulation. The light blue boxes represent the generic tools: experiments, atomistic simulation, and simulation of experiments. The dark blue represents the conceptual pathways leading to their quantitative connection, which in turn leads to the interaction and influence of atomistic simulation on experiment and vice versa.

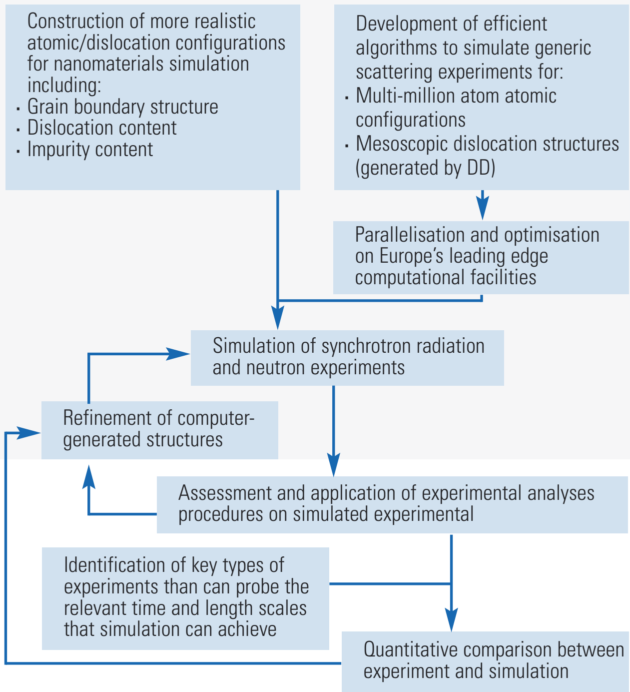


Fig. 2.5.3: Research roadmap for the implementation of the outlined strategy for the deformation of a nanocrystalline material.

Scope of strategy

The current strategy extends the multi-disciplinary approach taken in pure simulation (see section 2.5.1) to include within its scope:

- Simulation of experiments;
- Existing and emerging neutron and synchrotron experimental techniques;
- Modern and computationally intensive data analyses procedures.

This in turn expands on the class of tools needed for the validation and the self-benchmarking of modelling and simulation. By its very nature, the strategy is general and therefore flexible enough to encompass the wide class of nanomaterials and experiments available now and in the future.

2.5.3. RECOMMENDATIONS AND FUTURE OPPORTUNITIES FOR RESEARCH IN NANOMATERIALS THEORY/MODELLING/SIMULATION FOR LARGE TEST FACILITY EXPERIMENTS

European institute of excellence in "Nanomaterials – theory, modelling and simulation"

The challenging task of modelling and simulation of nanomaterials in connection with advanced synchrotron and neutron experimental techniques requires a concerted effort to advance theoretical techniques in parallel with the experiments. The optimal use of advanced synchrotron and neutron sources in science and technology of nanomaterials therefore calls for the development of an Institute of Excellence in Nanomaterials Theory, Modelling and Simulation. While such an institute may be broader in scope, synchrotron and neutron experiments pose the following requirements:

- Must be well connected to experimental groups working on advanced synchrotron and neutron techniques – (but must not necessarily be located at the site of a source);
- Must be multidisciplinary to cover physical, chemical, structural, materials specific and mechanical aspects of nanomaterials investigation;
- Could synergistically combine modelling and simulation of different experimental approaches e.g. electron microscopy and diffraction with synchrotron diffraction and spectroscopic techniques.

2.6. GENERAL CONCLUSIONS ON GENERIC CHALLENGES IN NANOMATERIALS RESEARCH – "GENNESYS SCIENCE CENTRES"

From the in-depth analysis of the generic challenges for the future fundamental research in nanomaterials science a detailed picture for the future role of the European synchrotron radiation and neutron facilities has emerged. The key conclusions and key recommendations are summarised as follows:

Key conclusions

- The future development and design of novel knowledge-based materials with properties tailored at the nanometre scale pose several challenges in all areas of fundamental research. The control of the functions as well as the long-term performance of new advanced materials architectures are directly linked to the microscopic understanding of the generic nanomaterials phenomena.
- In order to make a significant step further from current academic nanoscience efforts to a future application-oriented nanomaterials research, the future challenge is to investigate nanomaterials structures during operation (in-situ), in a destruction-free way and under relevant environmental and (future) industrial conditions.
- While the standard nanoscience tools (STM and AFM) are and will be most helpful for model nanostructures at free surfaces, they are not applicable in complex reaction chambers, for the characterisation of buried interfaces, for the monitoring of subtle structural details as strain and composition profiles which determine the performance and the degradation of a given nanostructure.
- A European strategy on the advancement of nanomaterials research and technology must develop sustainable and coordinated research efforts to address these generic challenges. In this effort, the European synchrotron radiation and neutron facilites must play an important role, since they carry the necessary in-situ analytical potential.

Key recommendations

- The European synchrotron radiation and neutron facilities must develop and optimise the necessary analytical tools to the future needs in nanomaterials research and must prepare the necessary scientific and technological infrastructure for the non-destructive in-situ analysis of nanomaterials and nanodevices.
- It is vital that the information on the already available and future possibilities at the European synchrotron radiation and neutron facilities for the investigation of nanomaterials phenomena is to be communicated between the different communities in much better way.
- Coordinated European research programmes need to be implemented integrating the European synchrotron radiation and neutron facilities for the in-situ and non-destructive characterisation of nanomaterials structures, phenomena, and functions providing a precise and systematic database of nanomaterials structures as input for improved nanomaterials models.

Three research areas have been identified requiring focused attention in the next 10 years:

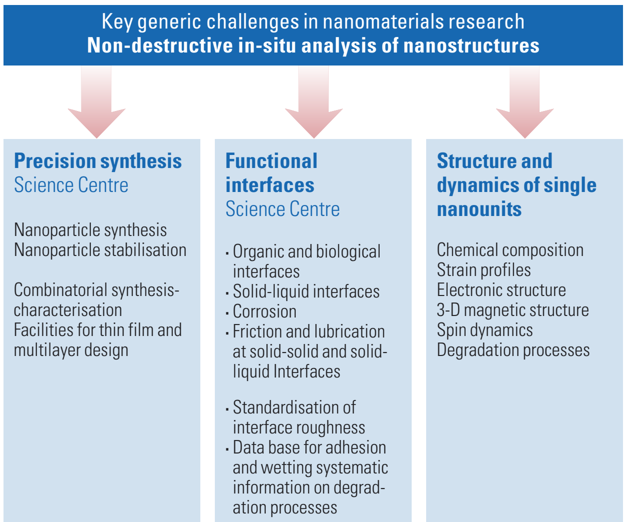


Fig. 2.6.1: Major areas of fundamental research for generic nanomaterials challenges.

- **SCIENCE CENTRE precision synthesis of nanomaterials**
  The future need to get a much better and more direct microscopic control of the growth, synthesis and design of nanomaterials, is a key challenge on the European roadmap for the advancement of nanomaterials research and development. It is necessary to create a new Science Centre at a European Synchrotron/neutron facility for the **"precision synthesis of nanomaterials"** which substantially advances our knowledge in:

· The precise synthesis of tailored nanoparticles (in-situ information on size, shape, internal structure during nucleation and growth);
· The controlled growth of functional nanounits on substrates (particularly for catalytic applications);
· The advanced growth of thin films and multilayers (in particular organic and biological systems and for nanoelectronic applications);

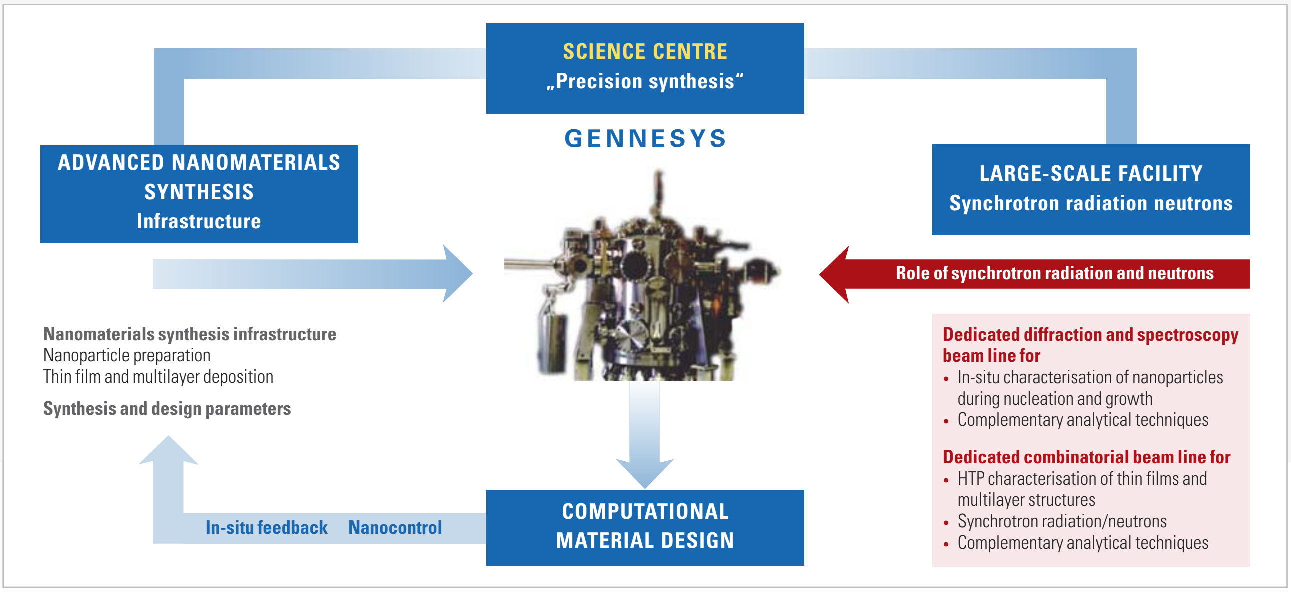


Fig. 2.6.2: Structure of a science centre on “precision synthesis”.

The Science Centre should include the following capabilities:

- Integration of experts in the synthesis of nanomaterials, experts in the in-situ analysis of the structure and property of nanomaterials and experts in materials modelling.
- In-situ full characterisation of the emerging nanostructure during the synthesis process at all stages of the process by real-time diffraction and spectroscopy allowing direct feedback to the relevant synthesis parametres (via a material modelling link).
- Ultrafast diffraction and spectroscopy studies of the initial nucleation process.

- **SCIENCE CENTRE functional interfaces**

  The microscopic understanding of the structure of and processes at functional interfaces has been discovered as a key barrier for the future design of nanomaterials. Thus, major effort has to be devoted to get this important structural information under nanocontrol.

  Synchrotron radiation and neutrons play a key role, since these probes are able to access buried interfaces or surfaces under extreme conditions.

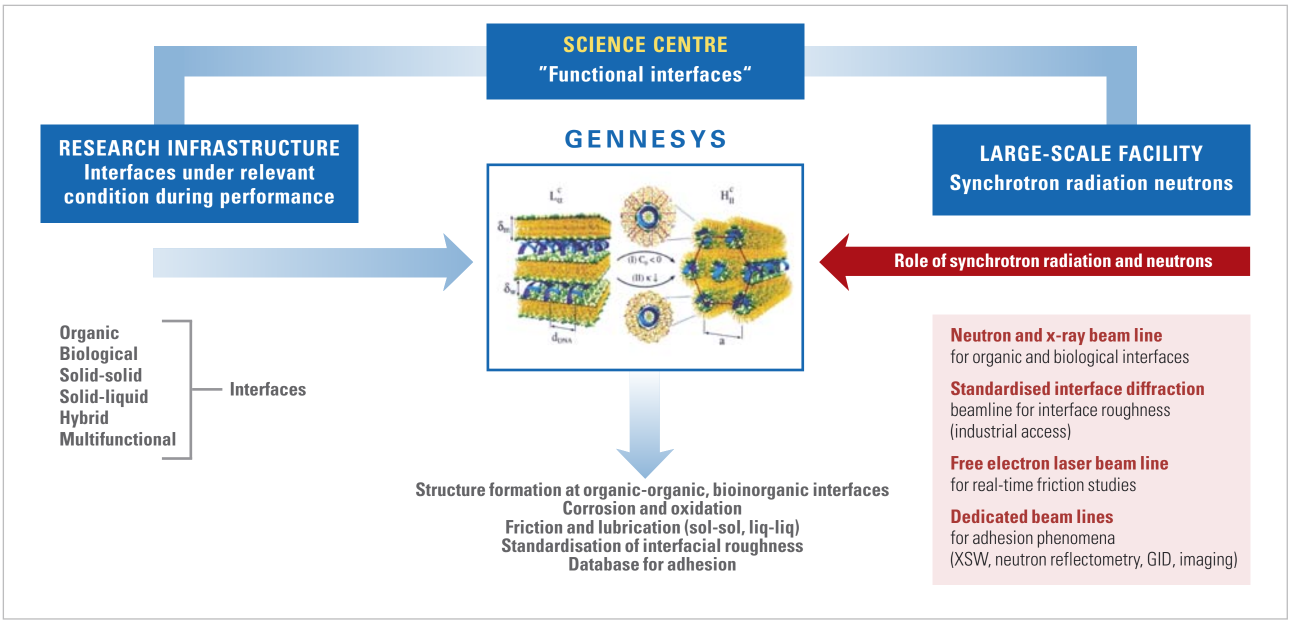


Fig. 2.6.3: Structure of a science centre on “functional interfaces”.

In the future particular focus should be on:

- In-situ studies of the structure and structure formation at organic and biological interfaces (with a focus on the first monolayers);
- The in-situ real-time study of (electro-) corrosion processes;
  The analysis of friction and lubrication on the atomic scale and at the relevant time scale;
- Standardisation: interface and thin film properties: roughness, elastic behaviour;
- Systematic in-situ studies of degradation, corrosion, friction (sol-liquid, sol-solid);
- Systematic measurements of adhesion energies (adhesion database) by combined interface sensitive diffraction-spectroscopy experiments.

Both science centres should work together closely with regular exchange of scientists and technology. Both science centres should stay in close contact to industry (as new electronics and new catalysors).

- **Research consortium: structure and dynamic of single nanoparticles**

  The microscopic insight into all structural features of a single nanounit is an enormous challenge. Currently, only tunnelling probes are able to select single nanounits and provide local information. However, the emerging need of nanomaterials design is the analytical access of internal structural details of individual nanounits under different operation conditions.
  Thus, a major task for synchrotron radiation and free electron x-ray laser facilities is to design and provide stable nano x-ray beams and fully coherent x-ray beams for the destruction-free investigation of the relevant local properties of the designed individual nanounits. European research consortia consisting of experts in nanoparticle design, experts in the use of x-ray nanobeams and coherent x-ray beams must work together to develop the necessary technology and know-how to enable in-situ structural investigation of arbitrary nanounits under arbitrary conditions.

  This research consortium should work in close contact with the science centre "precision synthesis", since the new analytical methods developed in the area of nanobeam diffraction and spectroscopy could have an impact on the in-situ control of nanoparticle synthesis.

3. SPECIFIC CHALLENGES FOR NANOMATERIALS DESIGN

3.1. OVERVIEW

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[Affiliations chapter 12]

The term 'nanomaterials' describes materials that are composed of structural elements whose characteristic size in at least one dimension is of the order of a few nanometres. Nanomaterials thus include nanometre-sized microstructures, suspensions of nanometre-sized crystallites, high surface area materials, carbon-based materials (such as nanotubes), materials with nanostructured surface regions, nanometre-sized thin films, and nanostructured devices.

Nanomaterials can be divided into the following groups:
- Materials and devices with reduced dimensionality in the form of isolated, substrate-supported or embedded nanometre-sized particles, thin wires and thin films;
- Materials and/or devices in which the nanometre-sized microstructure is limited to a thin (nanometre-sized) surface region of a bulk material;
- Bulk solids with a nanometre-scaled microstructure where either the atomic structure and/or chemical structure varies on the atomic scale throughout the solid, or where the microstructure consists of nanometre-sized building blocks.

Since the properties of solids depend on their chemical composition, atomic structure and microstructure, nanomaterials may exhibit properties that differ greatly from those of conventional polycrystalline materials. They may show very high or no ductility, depending on the energy stored in the interfacial regions. The potential benefits achievable by microstructural refinement/optimisation are well illustrated by nanocomposites used as hard metals in the cutting industry, and oxide nanocomposites for catalysts.

Conventional manufacturing methods are often not well-suited for nanomaterials as they can be incompatible with achieving the desired material properties. Therefore, novel methods for handling nanomaterials and converting them into engineering components are needed.

This chapter on nanomaterials design examines metals, ceramics, polymers and composite systems that are used either as functional (e.g. for their magnetic or sensing properties, electronic materials, superconductors) or as structural materials (e.g. light-weight, high temperature, high-strength materials). The range of nanomaterials applications is illustrated in Fig. 3.1.1. Particularly exciting are the:
- Opportunities to advance the performance of functional materials by rearranging matter at the molecular or atomic level. Special importance is seen in the control of quantum mechanics and in the use of proximity effects.
- Prospects for advanced structural materials that have been microstructurally refined and stabilised at the nanoscale level.

Functional materials

Solid state physics is poised for a paradigm shift: from bulk average behaviour to nanoscaled tailored structures (100 to 10,000 atoms). Accurate prediction of complex materials properties at small sizes and fast times is possible, if sufficient effort is invested in systematic and quantitative correlations of the structural and physical properties of nanoscale solids.

Breakthroughs using neutrons and synchrotron radiation techniques for future functional materials are expected by the control of the nanofabric of for example:

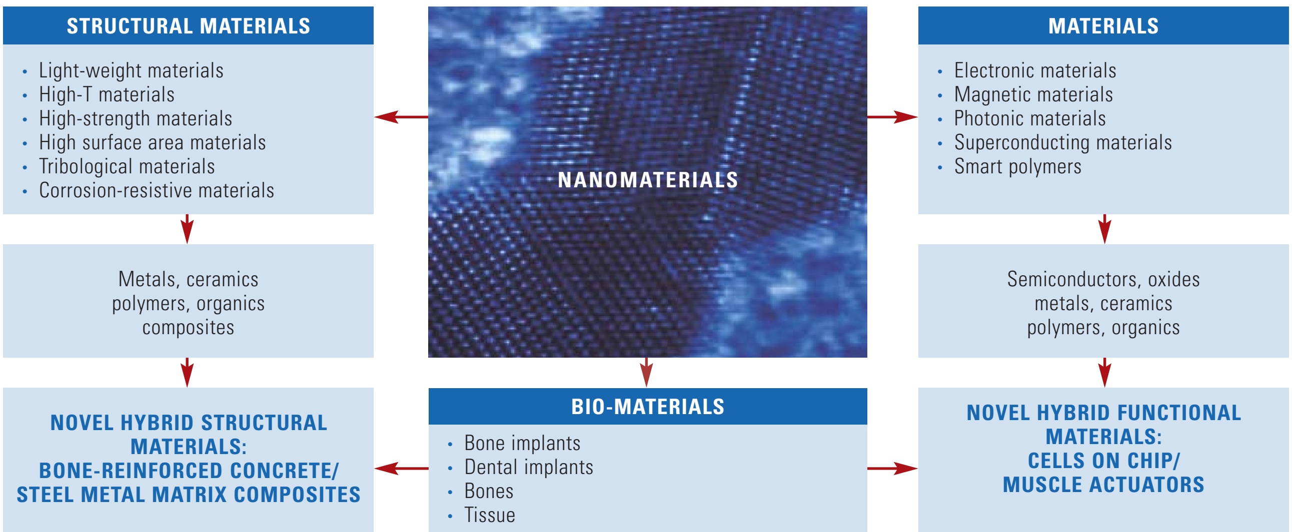

Fig. 3.1.1: Overview: nanomaterials.

- Magnetic nanomaterials: to use controlled nanoscaled magnetic structures to develop high density storage media; to use "spintronics"; to beat the super paramagnetic limit;
- Carbon nanomaterials: detailed information on atomic structure; elucidation of electronic/chemical properties;
- Polymers: functionally defined comb-shaped supramolecules based on hydrogen bonding; robust controlled ionic self-assembly.

Structural materials

Nowadays, many structural materials have reached a high degree of scientific and technical maturity. Progress has thus plateaued in many areas, with incremental changes now being achieved. To master decisive steps in future developments of structural materials, new approaches are needed, including:

- Control of microstructural development during processing on the nanoscale;
- Understanding and control of damage accumulation/failure below the continuum level;
- Production of stable 20 – 500 nm grain sizes to obtain unprecedented properties in strength, toughness and fatigue resistance of bulk metals and ceramics;
- Tools for the prediction of materials properties for complex nanoscale structures.

A key feature of the nanomaterials 'revolution' is that it cuts across an enormous range of products and applications in industry, manufacturing, healthcare, and public services (Fig. 3.1.2). The impact of nanomaterials will be of great importance in meeting future challenges for the benefit of society in the European Union and worldwide.

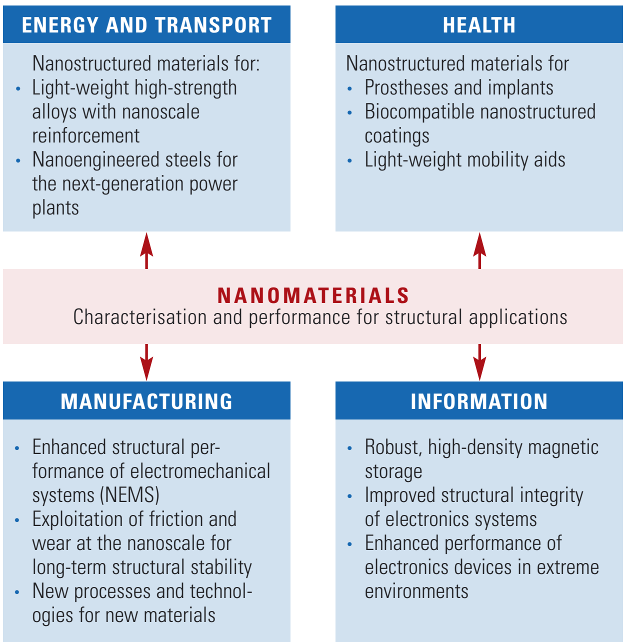

Fig. 3.1.2: The potential impact of nanomaterials.

Future research needs/targets:

Future research on nanomaterials will need to strengthen the European capability and potential to:

- Create and fabricate nanomaterials with reproducible, manageable microstructural characteristics;
- Handle and assemble these materials into bulk materials and devices;
- Derive new testing methods for diagnosing defects and/or damage in nanomaterials and components;
- Introduce new design concepts for nanomaterials and nanoscaled devices;
- Devise concepts for numerical simulations of nanomaterial response to processing and loading operations.

There is a wide range of techniques, using neutrons and synchrotron radiation, which will contribute to these research areas. Some examples are given in Fig. 3.1.3.

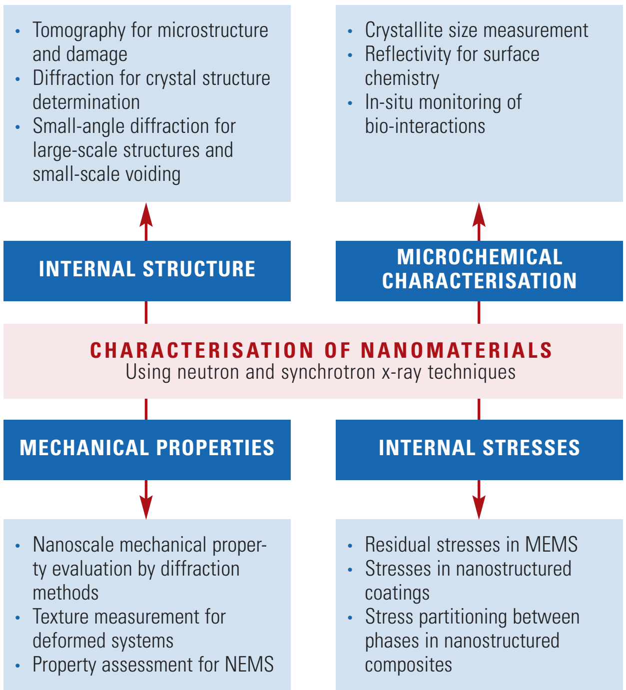

Fig. 3.1.3: Nanomaterials research: the application of neutron and synchrotron x-ray methods.

3.2. MATERIALS SPECIFIC CHALLENGES FOR THE SYNTHESIS OF NANOMATERIALS

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3.2.1. STATE-OF-THE-ART SYNTHESIS AND PROCESSING METHODS FOR NANOMATERIALS

Approaches to the synthesis of nanomaterials can be divided into two main classes:

- Top-down-approaches: a bulk material is restructured (i.e. partially dismantled) to form nanomaterials.
  Top-down methods are usually conceived as deterministic fabrication strategies. The aggressive scaling of integrated circuits in recent years can be considered the greatest success of this paradigm. For top-down methods, the challenges increase as devices size is reduced and as deterministic designs become larger and more complex.

- Bottom-up approaches: the nanomaterials are assembled from basic building blocks, such as molecules or nanoclusters.
  Basic building blocks, in general, are nanoscale objects with suitable properties that can be grown from elemental precursors. The concept of the bottom-up paradigm is that the complexity of nanoscale components should reside in their self-assembled internal structure, while requiring as limited action as possible from the macroscopic world. Also, deterministic assembly of nanocomponents over large areas is difficult and expensive. Hence, the organisation of bottom-up building blocks into some kind of hierarchical architecture must again rely on some form of self-assembly (inspired for example by protein synthesis) or, more frequently, on processes characterised by a significant level of randomness.

Methods for nanomaterial preparation can also be classified depending on the phase in which the synthesis reactions take place (gas, liquid or solid phase).

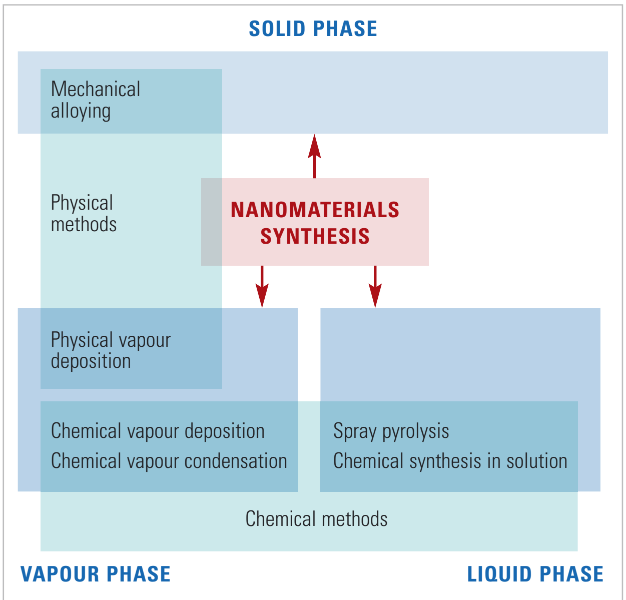

Fig. 3.2.1: Classification of nanomaterials synthesis.

Chemical methods usually employ reactions either in the liquid phase or in the gas phase, whereas physical methods are generally carried out either in the gas phase or entirely in the solid phase (i.e. mechanical milling). In some cases, these distinctions vanish as some processes involve reactions in several phases at once (i.e. the vapour-liquid-solid growth of nanotubes/nanowires onto substrates, or the solution-liquid-solid growth of nanorods/nanowires in solution).

- **Vapour phase reactions** can be classified into three main classes:
  - Physical vapour deposition;
  - Chemical vapour condensation;
  - Chemical vapour deposition.

Physical vapour deposition	Physical Vapour Deposition (PVD), Inert Gas Condensation (IGC), Cryogenic Melting (CM), Arc Discharge (AD), Hydrogen Plasma Melting Reaction (HPMR)
Chemical vapour deposition	Thermally-activated Chemical Vapour Deposition (CVD), Plasma-Enhanced Chemical Vapour Deposition, Laser-Assisted Chemical Vapour Deposition
Chemical vapour condensation	Thermally Activated Chemical Vapour Condensation (CVC), Microwave Plasma Process (MPP), Combustion Flame Pyrolysis, Laser Pyrolysis
Spray pyrolysis	Conventional Spray Pyrolysis, Electrospray, Low-pressure spray pyrolysis, Salt-assisted spray pyrolysis, Ultrasonic spray pyrolysis
Chemical synthesis in solution	Growth in microemulsions, Growth in presence of surface stabilising agents, Conventional Hydrothermal methods, Hydrothermal synthesis in supercritical solvents, Sol-gel methods, Sonochemical methods, Electrodeposition methods
Mechanical alloying	Mechanical alloying

Table 3.2.1: Examples of synthesis methods grouped by category.

In general, chemical vapour condensation routes refer to vapour-phase chemical approaches to nanopowders, whereas chemical vapour deposition refers in general to deposition routes of thin nanocrystalline films. The main advantage of gas phase is that the following properties can be attained: small particle size, narrow size distributions and high purity of nanoparticles/nanocrystalline films. Some of these methods, however, still remain remarkably expensive.

To date, spray pyrolysis (a liquid-to solid conversion process), is the only liquid phase methods that is low cost and amenable to large-scale production, since it is based on a continuous operation process.

- **Solid phase** reactions essentially involve mechanical alloying:
- **Nanocomposite processing approaches** aim mainly at consolidating nanopowders into bulk shapes, or transforming large grain materials/composites into nanosize grain material/composites.

Processing groups can be categorised as either:
- Mechanical or thermomechanical (plastic deformation, hot-pressing, sintering, etc.);
- Non-equilibrium processes (micro-wave/spark-plasma sintering, spray processing, etc.).

3.2.2. UNFOLDING THE FUTURE OF NANOMATERIALS SYNTHESIS

It can be foreseen today that two ages will be faced as long as nanomaterials will fully develop their technology potential. These will be referred to herein as the "nanobulk" age and the "nanoworld" age. Conceptually, they lie at opposite extremes, since they reflect respectively the two major paradigms of nanofabrication. Yet, an overlap between the two ages is predicted to be possible, because there are frameworks where they do not necessarily exclude each other, but appear rather complementary.

a) The nanobulk age

In the nanobulk age, which has already begun and will further develop in the coming 10–15 years, the benefits of nanomaterials will be exploited at the macroscale. In this age, a nanomaterial is not a single nanoparticle, nanowire, or DNA strand, but rather a human scale object (solid, liquid or even gas) whose novel properties at the macroscale are to be determined by its nanoscopic internal structure.

To clarify this, a few realistic applications of bulk nanomaterials are listed below:
- Cosmetics containing nanoparticles can be found already on the market;
- Healthcare: nanoparticle suspensions or solutions to be injected into living tissues to help diagnostics or drug delivery;
- Energy: large-scale nanostructured materials, thanks to their high surface to volume ratio, are potentially superior triggers to enhance every type of surface- or interface-based chemical reaction, i.e., reactions for energy generation, conversion and storage;
- Automotive/infrastructure: composite materials containing nano-objects with extraordinary mechanical properties can result in novel outstanding performances, enabling for instance the application of novel coatings with unprecedented resistances.

From this short list, it is evident already that nanomaterials in a bulk (a cream, a pill, a coating on an aircraft wing) do not require individual manipulation, nor do they require any sort of periodic order reminding of crystallographic lattices. These random ensembles of nanostructures call for synthesis methods inspired by the bottom-up paradigm, and thus bottom-up growth techniques will inevitably play a dominant role in the nanobulk age.

Consequently, future challenges to tackle in the next 10–15 years are:
- High costs associated with the productions large quantities of uniform nanopowders limits the use of nanoscale materials in several practical applications today. There is a need for the development of more cost-effective, efficient and environmentally-friendly synthetic processes of large amounts of nanoparticles;
- There will be a need for novel methods to store and handle nanopowders prior to their processing in order to reduce or avoid contamination, nanoparticle degradation, and aggregation;
- Consolidation techniques to nanocomposite materials will need to achieve higher efficiency in full consolidation of nanopowders while retaining nanometre grain sizes and full inter-particle bonding;
- Microbial approaches to the synthesis of nanoparticles might lead to cheap re-usable bio-reactors that will deliver certain classes of nanomaterials with a high specificity.

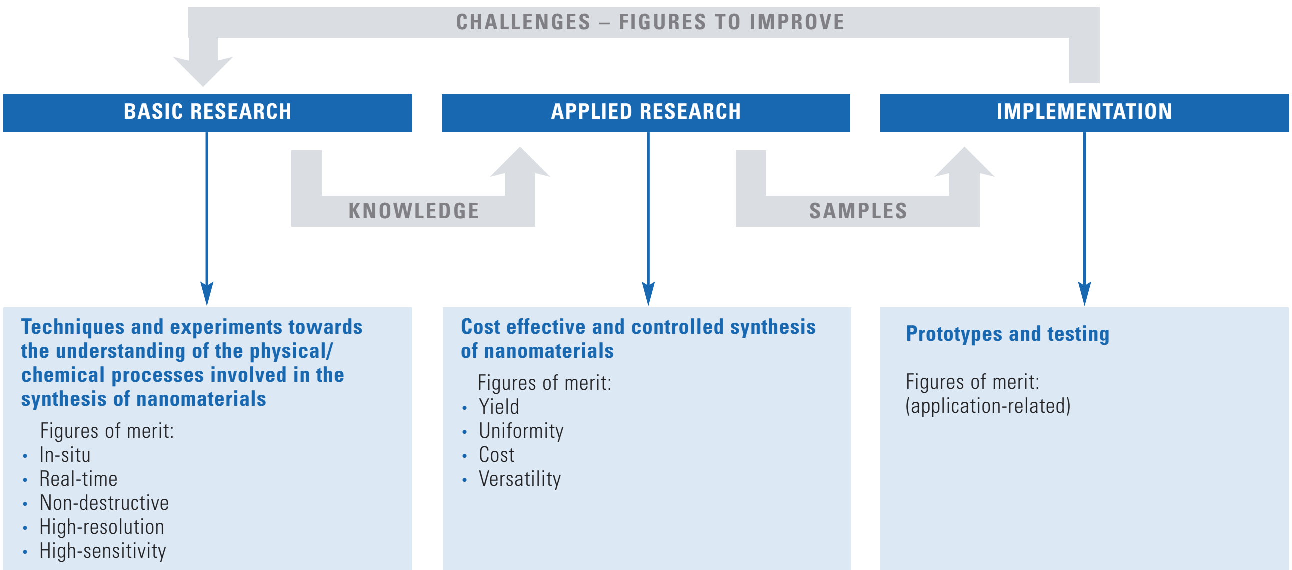

Fig. 3.2.2: Research and technology development in the nanobulk age.

It is predictable that research and technology development in the nanobulk age will follow the scheme summarised in the next diagramme (Fig. 3.2.2).

From the implementation point of view, the most important figure is yield, as discussed above. If nanomaterials are to be implemented on macroscale object, macroscale bodies, or macroscale power stations, cost-effective mass-production of nanomaterials is essential. According to tolerances, other important parameters will come into play such as uniformity, purity, toxicology, stability. Now, applied research will try to provide samples targeting these requirements, using relatively cheap and environmentally-friendly synthesis facilities.

Pioneering examples in this framework are the growth of semiconductor nanocrystals via solution processing, and the vapour-phase bulk production of carbon nanotubes via arc-discharge or CVD. These approaches highlight the scale-up potential of both liquid-phase and vapour-phase techniques for mass-scale nanomaterial synthesis, though some challenges still need to be addressed:

- **Development of microstructured reactors for large-scale continuous synthesis of nanomaterials in solution**

The fabrication of nanomaterials in the liquid phase is becoming more refined and thus more demanding. Microfluidic-based reactor devices are demonstrating a much higher degree of accuracy than classical batch reactors in chemical synthesis, allowing one to rapidly change temperature, flows, and concentrations. Future synthesis approaches to solution-grown nanomaterials will rely heavily on reactors based on microfluidic channels in which it will be possible to control precisely the chemical and physical properties of the resulting nanomaterials. Critical points will be the choice of materials by which the various parts of these microreactors will be built, as the synthesis conditions for growing nanomaterials can be very harsh. The possibility to realise large temperature gradients in specific regions of the microchannels will allow control of the nucleation and the growth events at a level that cannot be attained currently. Heating and cooling will therefore be possible at very fast rates and with a much lower consumption of solvents, with clear environmental and economical advantages. This will be particularly useful for a series of nanomaterials (i.e. III-V and group IV semiconductor nanocrystals, various ceramic materials, and so on).

- **Cost-effective bulk production of nanomaterials via vapour phase**

Several vapour-phase growth strategies have been proposed to achieve large-scale production of nanomaterials, mostly focusing on one-dimensional nanostructures like carbon nanotubes or nanowires. In many cases, a metal catalyst particle is needed to trigger the growth. With process temperatures usually exceeding 800°C, Au, Fe, Ni, Co are mixed to the precursor vapour either by thermal evaporation or laser ablation. NWs are collected from the furnace reactor in the form of wool-like bundles. To optimise the cost-per-run ratio, continuous collection of nanomaterial bundles (e.g., fibre "spinning") will be crucial. There is a need, moreover, to avoid the metal contamination potentially arising from the residual catalyst particles. Removing the catalyst post-growth may require complex and expensive purification treatments. Shape-separation of as-grown bundles requires further processing. Future research in this direction will aim to engineer and optimise the synthesis in order to achieve a 100% yield of the desired nanostructure morphology.

- **Development of more efficient and environmentally-friendly synthetic processes based on biochemistry**

The development of biochemical routes for the synthesis of nanomaterials might open new perspectives in the field. Heavy metal resistance and detoxification strategies of various strands of bacteria could be exploited for the controlled synthesis of different types of nanomaterials, especially those based on toxic chemical species, with the clear advantage of carrying out reactions at much lower temperatures compared to the actual temperatures (especially for the case of vapour-phase growth). Also the use of toxic and expensive surfactants/precursors can be avoided.

Given the simplicity and low cost of many bottom-up growth facilities being actively developed in the "applied research" sector of the nanobulk age, it would be tempting to optimise the synthesis processes by iterative and empirical attempts. Although empirical investigations are indeed possible and sometimes very effective, solving specific issues and unveiling performance-limiting factors will call for a deep understanding of the chemical and physical processes involved in the growth. Here is where "basic research" and fundamental characterisation techniques begin to play a critical role. Even if the ultimate scope is producing trillions of nominally-equivalent nanostructures, the focus of basic research is the study of the synthesis of an individual nanocomponent (or, at least, of the average nanocomponent):

- To understand how it is formed and how the process can be better controlled;
- To understand why two nanocomponents may be nominally-equivalent but not fully equivalent;
- To spot at the root potential failures during synthesis, which are eventually responsible for implementation challenges.

In this direction, the best characterisation strategies are based on in-situ, real-time techniques. This calls for non-destructive, high-resolution means of characterisation that can follow the evolution of the synthesis process while it is taking place. Many techniques are possible (Raman, optical absorption and fluorescence, x-ray diffraction, transmission electron microscopy, etc.), including neutron scattering, high-resolution and high-sensitivity EXAFS or XPS based on synchrotron radiation.

It is also worthy to mention the need for theoretical and computational support. Several tools for modelling nanomaterials growth are now available, ranging from classical simulations, to density functional theory and molecular dynamics. The main challenge is combining the atomistic insight of DFT or MD with the large temporal and special scales necessary to fully describe the growth process. Novel linear scaling DFT techniques, such as ONETEP, or hybrid "learn on the fly" methods are now becoming available. These methods, if properly and efficiently implemented, will allow for a multi-scale atomistic and mean field investigation of the growth mechanisms.

b) The nanoworld age

The nanoworld age is expected to unfold 15–40 years in the future, thus it is a much longer-term vision than its nanobulk counterpart. The nanoworld paradigm no longer considers nanocomponents as "nominally-equivalent within tolerance", but aims to take advantage of the natural or induced diversity among nanoblocks. Stretching the discussion on more figurative terms, one could say that while drama is the official game of the nanobulk age (many equivalent chips are needed), the nanoworld age is more oriented to chess (where individual different pieces have different functions). Treating nanocomponents no longer as a mass but as individuals is obviously more challenging. It implies that any proposed synthesis strategy should have a very precise and independent degree of control over the structure of every single nano-object and/or the location where to assemble or grow it. The randomness of nanobulks must be replaced with a deterministic control at the nanoscale.

As for the human world, differentiation means more intelligence. In fact, foreseeable applications for the nanoworld approach to nanofabrication will produce small objects, taking the advantages of nano-as such (high-integration, low power consumption, non-invasive monitoring). This goes in the direction of supporting novel computing resources, with complex nanomachines possessing a sort of embedded intelligence. Applications span from neural computing, sensing and ambient intelligence, nanomachines for self-surgery and intelligent drug delivery.

Technologically, the development diagramme for the nanoworld age is similar to the nanobulk one (Fig. 3.2.3). However, basic research and applied research will inevitably merge into the same block. This is because the fabrication of samples will no longer target mass production or cheap strategies. The emphasis will shift towards fabricating an "intelligent" nanoworld, whatever its cost. Thus, highly-sophisticated synthesis and characterisation facilities will both be needed. In this framework, empirical research no longer pays off, and the fundamental understanding of the process becomes priority.

Owing to the deterministic character of the nanoworld, top-down methods will rise again in popularity and will continue to play an important role within their intrinsic limitations. Bottom-up strategies, improved and optimised during the nanobulk age, will ultimately take over certain aspects (but not all) of top-down processing via intelligent self assembly. "Hybrid fabrication" (intended as a mixture of top-down and bottom-up processing), will represent the most popular keyword of the nanoworld age.

As an example, we can consider the potential role of chemical vapour deposition (CVD) for hybrid fabrication of non-equivalent nano-objects. CVD is a very popular synthesis technique for nanomaterials, and probably the most investigated for 1-D nanostructures. As explained before, a metal nanoparticle is often required to favour selective decomposition of the precursor gas, and the consequent nucleation of substrate-bound 1-D nanostructure. By patterning the catalyst via top-down methods on oriented crystalline substrates, defined and oriented arrays of nanowires or nanotubes can be fabricated. Within a single growth run, nanomaterials with different properties can be produced simultaneously, driven by the initial state of the catalyst. Thicker catalyst particles will yield thicker nanowires, catalyst alloys will produce nanowires with different doping, etc. This highlights the potential of the hybrid approach for the realisation of a variety of nanosystems (or nanoworlds, for consistency), where active components will be no longer manufactured but grown from point to point in an intelligent fashion.

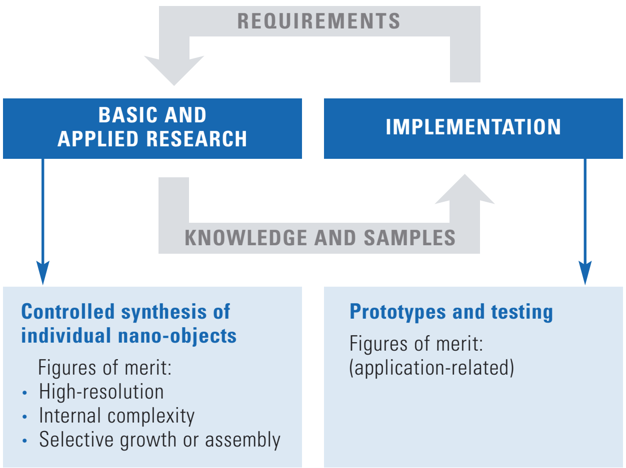

Fig. 3.2.3: Research and technology development in the nanoworld age.

3.2.3. IMPORTANCE OF NEUTRONS, SYNCHROTRON RADIATION AND FEL IN THE FUTURE DEVELOPMENTS OF SYNTHESIS AND PROCESSING TECHNIQUES

To exploit the full potential that nanomaterials offer, a non-destructive structural and morphological characterisation is required. Most of the characterisation techniques routinely applied to micrometric materials, namely x-ray or neutron diffraction, extended x-ray absorption fine structure, small angle x-ray or neutron scattering, cannot be directly used – unaltered – to these smaller sizes, both during data acquisition stage and data treatment.

Indeed in nanomaterials, due to the extraordinary large surface rule surface atoms percentages (50–75%), the process of minimisation of the surface energy leads to important strain contributions and/or surface atoms reconstruction. This can determine novel and unexpected atomic arrangements with respect to the bulk parent lattice, causing dramatic effects on other physical or chemical attributes.

The precise determination of the long- and medium-range order in nanocrystalline powders as well as in nanoparticle single crystals and/or the existence of local distortion (strain) inside a single nanocrystal, pose fundamental need in the research of the coming years and require a revolution of synchrotron-based instruments:

- Using smaller nanoprobes with higher brilliance: longer beam line and/or novel focusing elements will allow to reach focused beam sizes below 20 nm;
- Enhancing the detection limits to reduce the quantity of scattering volume from ppm to ppb;
- Integrating elemental, chemical and structural characterisation at the same facility;
- Studying the materials under extreme conditions of pressure, temperature or high magnetic fields;
- Exploiting the coherence properties of the synchrotron beams to open the pathway for new imaging techniques, where the individual properties of a single nanocrystal rather than the statistical properties of a group of nanocrystals could be assessed.

Beyond synchrotron radiation, Free Electron Lasers (FELs) will provide a peak brilliance 1010 higher than the best synchrotron light sources available today and photon pulses of 1012 photons per femtosecond (fs). Intrinsically, the FEL has pulses of about 200 fs in length. On the fs timescale, it will be possible to observe the effects of the motion of the nuclei on the electronic structure in a molecule, in a solid, or the behaviour of an adsorbate on a surface. In pump-probe experiments, the development of the electronic states in a dissociating or desorbing molecule could be followed, giving insight into the transition states and the nature of barriers that determine the pathways for chemical reactions. The FEL will offer a fully transverse coherent beam with about 100 degenerate photons within the coherence volume.

Possible research areas of synchrotron, neutron and FEL radiation in the nano-bulk age will mainly include characterisation of as-grown nanomaterials. A step forward would be to upgrade purely-analysis-oriented beamlines to low-throughput growth reactors with built-in structural monitoring capabilities. This will provide unprecedented data and insights on the real-time dynamic of the synthesis process, a critical figure of merit for basic research. A few examples are proposed below:

- **Monitoring the magnetisation dynamics of nanostructures on the fs timescale**
  FEL's will enable studies of the magnetisation dynamics of small magnetic nanostructures and clusters on the fs timescale in conjunction with nm spatial resolution. This could be an important tool to monitor in-situ the growth kinetics of magnetic materials, especially those based on the combination of materials of which one or more is magnetic (i.e. core-shell based or heterodimers of nanocrystals). In this case, the rapid time evolution of the magnetic properties of nanoparticles during growth, due to the formation of surfaces and interfaces between different materials, could be monitored.

- **Characterisation of large-scale nanomaterials using neutrons**
  Small-angle neutron scattering has been exploited as a technique to determine particle size distributions in nanocrystal ensembles, with the advantage that neutrons are able to sample large sample sizes. In the age of mass-production of nanomaterials, this technique could ensure a representative integrated assessment of the entire nanobulk.

  As explained in the previous section, however, figures of merit will change for the nanoworld age. Precision will become more important than yield and cost, thus those facilities that for nanobulks only played a characterisation role toward a basic and fundamental understanding, could become the only possible pathway towards applied synthesis with nanoscale deterministic control. As examples, one may consider:

- **Nanolithography using soft x-rays**
  The realisation of materials with controlled features in the nanometre range presents an immense challenge for the future. With Free-electron lasers (FEL), feature sizes may be realised that are much smaller than those envisioned for the next step in industrial applications of EUV lithography (at 13.5 nm), corresponding to a wavelength limit as short as 1.2 nm. The FEL, in which high power is concentrated in an extremely narrow spectral range, will therefore, be an ideal source for top-down nanolithography.

- **Solution synthesis of nanoparticles using synchrotron radiation coupled with a microfluidic reactor**
  As of today, there are a few reports on the solution synthesis of colloidal nanoparticles using synchrotron radiation (mainly noble metals prepared in aqueous solution). In the future, this approach might be extended to the synthesis of nanoparticles in micro-reactor systems. High-energy x-ray beams focused into spots that are a few micrometres wide would deliver into a specific region along a micrometre channel the energy required to decompose chemical precursors and induce nucleation of nanoparticles.

This approach might represent a valid alternative to locally heating the microchannel in order to induce the same effects. Local heating at high temperatures (300–400 °C or higher) would present the disadvantage that large temperature gradients would be generated, imposing heavy and often unbearable stresses to the materials of which the micro-reactors are composed. Lower-intensity synchrotron radiation could probe other locations along the microreactor (i.e. further ahead in the microchannel) in order to monitor the nucleation and growth of the nanoparticles (i.e. by recording in real-time diffraction spectra).

- **Fabrication of nanomaterials using neutrons**
  It was recently found that the synthesis of novel carbon nanomaterials can be catalysed by neutron irradiation. A possible advance in this field will therefore include patterned-neutron-irradiation for selective synthesis of various types of nanomaterials, also including organic nanoparticles (i.e. polymer nanoparticles).

3.2.4. SUMMARY AND CONCLUSION

The synthesis of nanomaterials is a pivotal research field towards the development of any future nanotechnology. Presently, a variety of techniques are used to grow or fabricate nanomaterials of different size and shape, including physical and chemical methods in the vapour and liquid phase. In the near term, efforts will concentrate on achieving mass production of nanoscaled materials, whereas in the medium/longer term controlled differentiation of nanoblocks will receive increasing attention. The development of both visions is strictly linked to an improved understanding of the physics and chemistry beneath different synthesis mechanisms. It is therefore necessary to support those branches of basic research (including synchrotron radiation and neutron scattering facilities) capable of providing the required fundamental knowledge for nanomaterial growth and implementation. Upgrades of existing facilities to make them suitable for real-time, in-situ nanomaterial characterisation are an essential step in this direction. Without taking these actions, Europe will miss a forerunner opportunity to engage in a dynamic interaction with the industrial world as illustrated in Fig. 3.2.2 and Fig. 3.2.3.

3.3. STRUCTURAL NANOMATERIALS

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Structural nanomaterials fulfill two tasks. Firstly, they perform a classical structural function, for example in increasing the strength of a weld by exploiting nanoscale phase transformations to reduce the weld stresses. Secondly, structural nanomaterials are implemented in cases where structural strength is just one aspect of performance, as is the case for intelligent windscreen glass. In some cases, the structures are large (a self-healing aircraft wing) in others small (actuators in a microelectronic machine).

Many structural materials have reached a high degree of scientific and technological maturity. Progress has thus plateaued in many areas, with only incremental changes now being achieved. Significant steps forward demand new approaches based on design at the nanolevel.

In this foresight study, we focus on the benefits of nanostructural materials in the areas of metals, ceramics, composites and structural coatings: examples of these material classes and applications are shown in Fig. 3.3.1. The study aims to illustrate the insights and acceleration of product development that the use of neutrons and synchrotron x-ray beams can bring.

Research needs for nanostructural materials

New materials, such as nanotubes and nanopowders, as well as new processes, such as severe metal deformation, are delivering new and exciting nanostructures with outstanding structural properties. A wide range of these developments across the field of structural materials can be advanced either by today's, or by modestly improved, neutron sources and synchrotron instruments. A number of aspects providing future breakthroughs in microstructural design and properties will require advances in the methods for neutron and synchrotron experiments to be realised. Nanomaterials will definitely play an increasingly important role, but the rate at which this occurs depends on the extent to which we can accelerate the development cycles shown in Fig. 3.3.2 and Fig. 3.3.3.

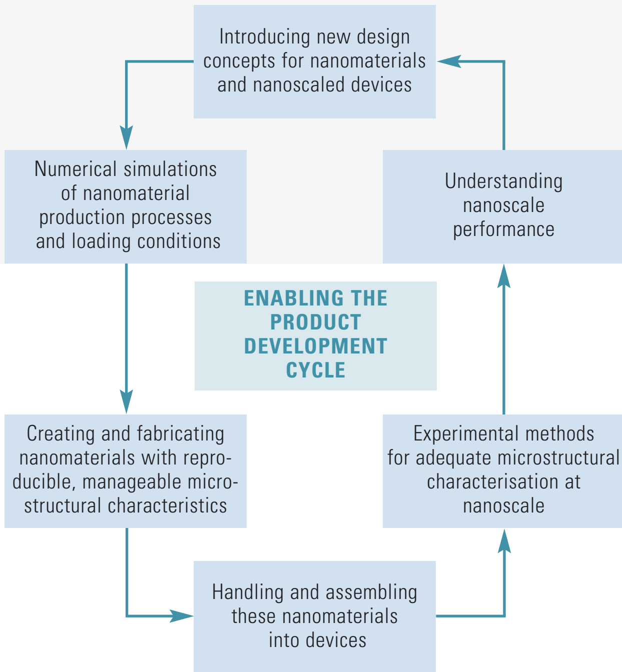

Fig. 3.3.2: Future research strategy for enabling the development of products based on nanostructural materials.

Neutron and synchrotron radiation techniques must play a major role in all aspects of the development cycle.

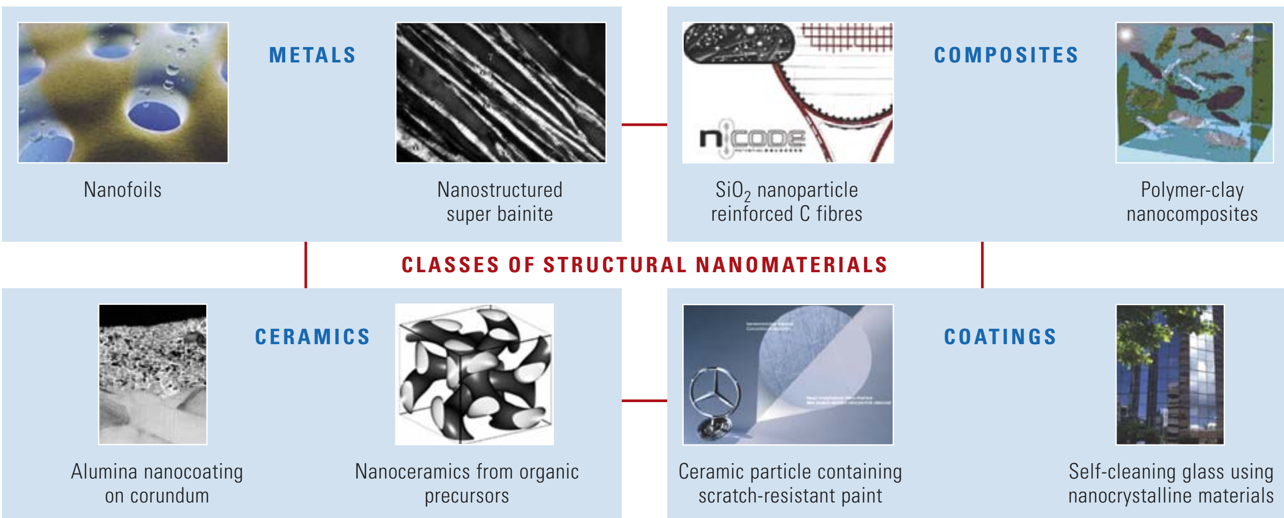

Fig. 3.3.1: Structural nanomaterials have the potential to provide drastic improvements in the range of materials we have at our disposal.

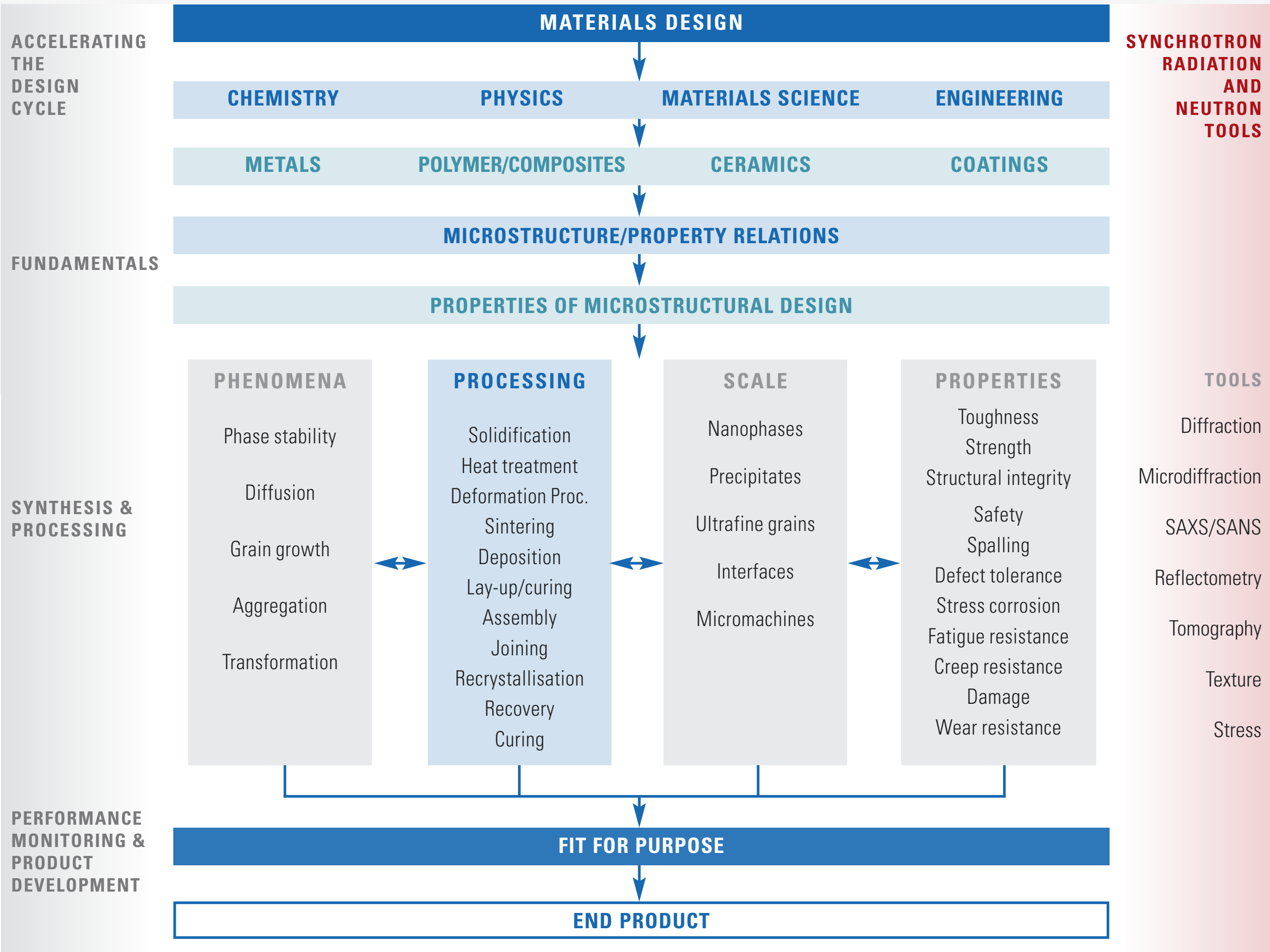

Fig. 3.3.3: This figure shows how neutron and synchrotron methods can accelerate the development cycle for the exploitation of nanomaterials.

3.3.1. METALLIC MATERIALS

Structural metallics include perhaps some of the oldest man-made nanomaterials: for instance, processes for optimising the structure of steels at a submicron scale have been applied empirically for centuries. There is a growing need for improved processing control and more reliable behaviour during application for existing classes and the next generation of materials. A key objective is to obtain unprecedented properties in strength, toughness and fatigue resistance of bulk metals and welds by the production of stable 20–500 nm grain sizes and the control of nanoscale precipitates and transformations.

Solidification processes

A basic understanding of the relationship between nanostructure and processing is essential in order to understand solidification. Solidification processes are extremely complex, requiring a plethora of neutron and synchrotron techniques to understand the dynamics of the process under realistic conditions and timescales.

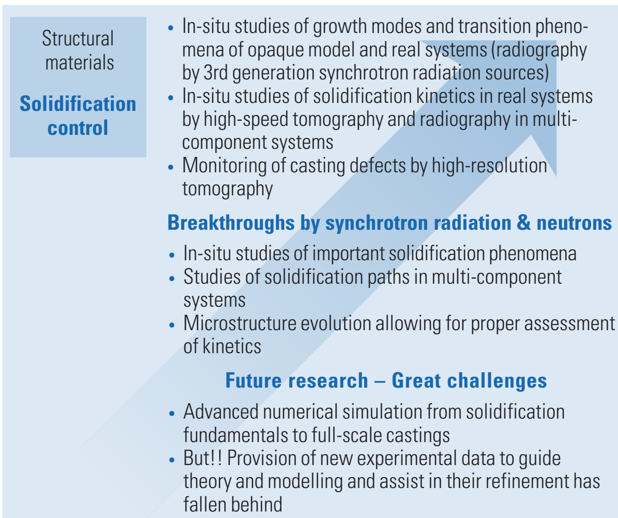

Fig. 3.3.4: Using neutron and synchrotron x-ray methods to understand and optimise solidification processes.

Numerical computer modelling for simulations covering the range from solidification fundamentals to the behaviour of full-scale castings has advanced considerably, whereas the provision of new experimental data which can guide theory and modelling, and ultimately assist in their refinement, has fallen behind. This gap therefore needs to be filled (see Fig. 3.3.4).
There are also challenges for subsequent thermomechanical processing (see Fig. 3.3.5).

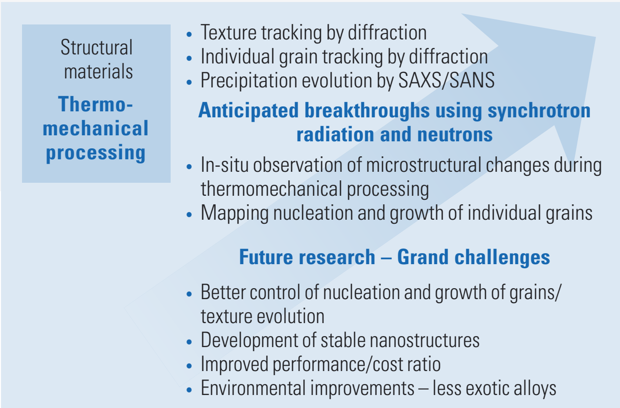

Fig. 3.3.5: Challenges in the future development of thermomechanical processing.

New metallic nanomaterials include intermetallics, ultrafine grained metals, smart metals and bulk metallic glasses (see Fig. 3.3.6).

- **Intermetallics** – offer, for instance, unrivalled potential for the elevation of operating temperature of metallic parts in aero-engines. While they have excellent high temperature strength, room temperature toughness and fatigue resistance remain problem areas. Nanostructuring may offer a solution, and the research challenges for such materials are shown in Fig. 3.3.7.

Diffraction studies, in real-time and at real or elevated temperature, should provide detailed information about the development of nanoscale intermetallic phases.

- **Ultrafine-grained metals** – offer improved properties without the need for exotic alloys that are uneconomic to recycle. Thermomechanical processing is the key to novel ultrafine-grained (UFG) metallics in many cases. In principle, such materials could have exceptional intrinsic properties like high ductility and high strength. It is conceivable that the technology can be expanded into the fabrication of large-volume aluminium and superplastic magnesium parts. Similar breakthroughs are expected from $\alpha+\beta$ Ti alloys with a submicrometre grain structure.

In-situ x-ray diffraction must be exploited to obtain a better understanding of UFG materials. A challenge, however, for using synchrotron radiation techniques in this area is the extremely high demand resolution imposed by finer grain sizes. However, grain structure evolution can be subjected to SAXS investigations even at very fine particle sizes. Development of dedicated experimental set-ups is needed for in-situ studies during the processing of UFG metals.

- **Smart metals** – can 'remember' their original shape (shape memory alloys) or have exceptional elastic properties (superelastic). These properties arise because of phase changes that can be thermally- or stress-activated. Some ferromagnetic alloys exhibit a huge strain of up to 11.4 % when exposed to moderate magnetic fields. Nanoscale twin boundaries propagate, driven by an externally applied magnetic field, though the volume of material, re-ordering the crystalline texture. Thus, a change in the macroscopic shape is achieved which is determined by to the anisotropy of the interatomic distances on the nanometre scale.

	INTERMETALLICS	SMART METALS	FINE GRAINS	GLASSES	TOOLS
Fundamentals	Exploiting phase diagramme	Stress- or environment-triggered transformation	Grain growth Recrystallisation	Crystallography Particle size	Crystallography Particle size
Synthesis and processing	Microstructural design	Phase management	Thermomechanical processing	SANS/SAXS Diffraction	SANS/SAXS Diffraction
Application	Controlling microcracking	Transformation property relations	Grain stability	Stress, diffraction tomography	Stress, diffraction tomography

Fig. 3.3.6: This figure shows how neutron and synchrotron methods can accelerate the development cycle for nanometallics.

The shape memory phenomenon is used in the set-up of a novel type of mechanical actuator that exhibits large strokes at relatively high operational frequencies up to 15 kHz. These actuators fill the gap between piezoceramic-based components with small strains but high operational frequencies, and the slow stroke magnets (see Fig. 3.3.8). These new actuators will underpin new technologies in the fields of very efficient ultrasound transducers; injection pumps, and magnetically-controlled valves that can replace the cam shaft of car engines and exhibit the required stroke-frequency characteristics for active damping components in aircraft. However, these alloys still suffer from limited operational temperatures and little ductility. In order to open the way for commercial applications, the structural and magnetic phase temperature stability ranges must be increased by specific alloy design.

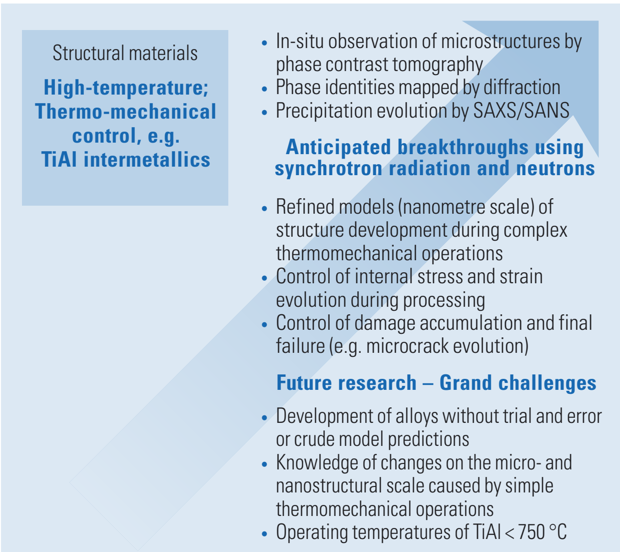

Fig. 3.3.7: Research challenges for improvement of the properties of high-temperature intermetallics.

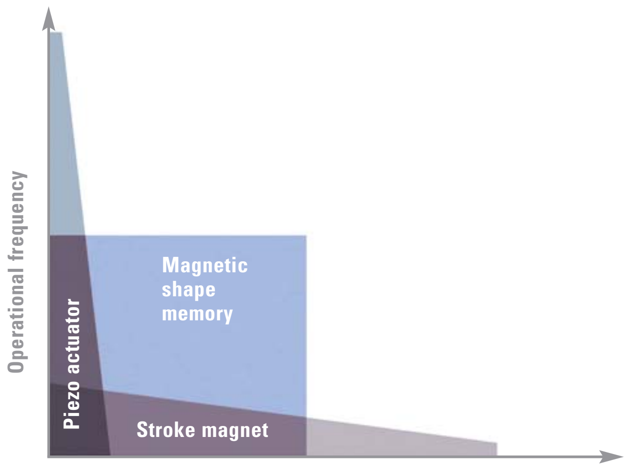

Fig. 3.3.8: Magnetic Shape Memory (MSM) alloys fill the gap between piezo-actuators and stroke magnets for the medium frequency range, together with medium strokes.

Neutron and x-ray diffraction have to be employed to monitor the extent of the above-mentioned phase stability ranges and provide key information about their structure, texture (preferred orientation) and internal stresses. For the class of magnetic shape memory (MSM) alloys, a complicated layered structure of nanoscaled periodicity is responsible for the extraordinary mobility of the nanosized twin boundaries. The domain arrangements within the alloy bulk can be characterised by neutron and high energy x-ray scattering methods due to the extremely high penetration depths.

- **Metallic glasses** – The last 10 years have seen the discovery of amorphous metal alloys that are glass-forming at cooling rates as slow as 1°C /s to as fast as 100°C /s. Bulk metallic glasses are twice as strong as steel, have greater wear and corrosion resistance, are tougher than ceramics, and yet have greater elasticity. Increased plasticity in amorphous/crystalline composites now promises new structural applications.

  It is imperative to probe the mechanisms of nanocrystallisation to obtain a better understanding of the thermal stability and glass-forming abilities of metallic glasses and to develop brand new nanocomposites (see Fig. 3.3.9). Using the principles of thermodynamics with kinetic calculations, it is possible to develop new materials from under-cooled liquids and metastable solid mixtures of alloys and ceramic phases within appropriate temperature/ internal energy constraints.

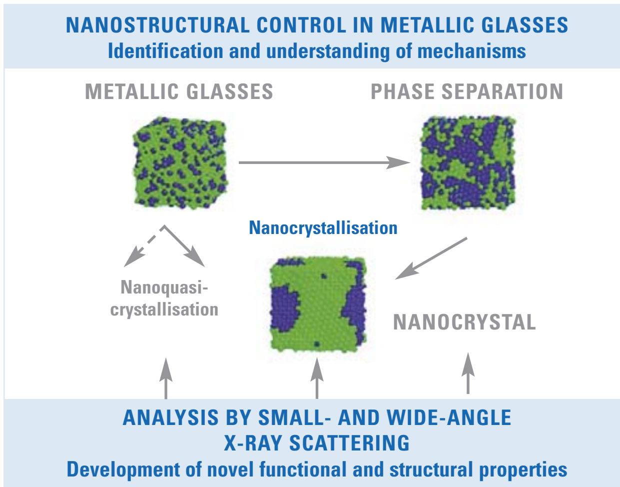

Fig. 3.3.9: The importance of nanocrystallisation for the development of bulk metallic glasses, and nanostructural analysis based on synchrotron radiation and neutron methods.

Synchrotron radiation has the unique ability to provide the tools for fast, accurate and in-situ characterisation of nanocrystallisation: small and medium angle scattering techniques are applied to examine the nanostructure formation in metallic glass materials.

Overall, the key challenges for the development of new and improved nanometallics can be summarised as in Fig. 3.3.10.

KEY NEUTRON & SYNCHROTRON RADIATION CHALLENGES

• Establish microstructural influences on intergranular strains during deformation →	In-situ diffraction →	New models of deformation
• Imaging of crack nucleation in fatigue and stress corrosion →	Micro-tomography →	Fracture mechanics
• Monitor rate of growth of individual recrystallising grains →	3-D x-ray microscope →	Refine recrystallisation theory
• 3-D monitoring of nano-precipitates or defects →	SANS/SAXS →	Metallurgy/ Structural integrity

Fig. 3.3.10: Metals: key neutron and synchrotron radiation challenges.

FUTURE APPLICATION AREAS OF SYNCHROTRON RADIATION AND NEUTRONS

Properties

- Fundamentals of crystalline deformation
- Distribution of nanoscale precipitates, dispersoids and defects
- Stress distribution between crystallites, phases and composite elements

Processing

- Growth of crystallites and grains during processing
- Development of process-induced internal stress and damage
- Active design of microstructure for properties
- Effect of processing methods on nanostructure

Products

- Residual and internal stresses in all phases, and at all length scales – from µm to cm – of nanostructured materials, composites and components, incl. MEMS and NEMS
- Damage accumulation in-service

3.3.2. METAL HYDRIDES

Hydrogen storage in a solid was first observed for the element palladium in 1866. Therefore, from a fundamental point of view, the Pd-H system is the best studied system even if its gravimetric density is low. Other elements show higher storage capacities e.g. titanium 4 wt%, magnesium 7.6 wt% with remarkably high volumetric densities. Hydrogen is dissolved as a proton in the crystal lattice of the metal and, therefore, the volumetric density in many cases exceeds that of molecular hydrogen in a liquid state. Nevertheless, elements showing a high gravimetric storage capacity usually possess a high temperature of dissolution, i.e. above 500 K or even higher, which is a major drawback for technical applications. The oil crises in the 1970's initiated large efforts to apply alternative energy carriers and, therefore, to find hydrides suitable for vehicles. At that time, the idea was to burn hydrogen in a conventional combustion engine, and Daimler-Benz AG even had a test fleet of 10 cars running in Berlin in the 1980's.

Indeed, several alloys based on inter-metallic compounds of a hydride forming element A and non-hydride forming element B have been developed which operate near room temperature and pressures between 0.1 and 1 MPa. These compounds can be divided into different families, AB_5 hydrides e.g. $LaNi_5$, AB_2 compounds related to Laves phase crystal structures, and AB hydrides, e.g. FeTi. However, the gravimetric storage capacity is below 2 wt% for all compounds operating at ambient temperature. Therefore, the storage of hydrogen in these hydrides would be a factor of 15 to 20 heavier than for gasoline and the development for these hydrides was stopped in the 1980's.

In the 1990's, the necessity to reduce atmospheric pollution and to avoid the greenhouse effect led to the development of fuel cells for mobile applications and prototype zero-emission vehicles. The ideal energy carrier for these vehicles is hydrogen. This initiated new research activities on hydrogen storage devices. Besides the classical storage of hydrogen pressurised in tanks or liquefied in cryogenic vessels, room temperature low pressure storage in solids has huge advantages. High pressure or cryogenic vessels can only be constructed with a very limited flexibility concerning their shape, whereas the container of a solid storage material may possess any kind of individual shape and, therefore, is comparable to the present gasoline tank.

Owing to the higher efficiency of fuel cells compared to combustion engines, the minimum gravimetric storage capacity requirement may be not so strict anymore and was set for example by the DOE to 6.5 wt%. However, the hydrogen should be released at temperatures compatible with the waste heat of fuel cells, i.e. below 370 K. One approach was to use the high storage capacity of magnesium and reduce the desorption temperature by preparing nanostructured composite materials with additives acting as catalysts. Despite many efforts, a reduction below 470 K seems to be impossible. Alkali metal aluminium hydrides have long been known to possess a high storage capacity and a high dehydriding temperature.

This situation changed when Bogdanovic and Schwickardi showed that with titanium doping, the temperature can be reduced to 420 K and a reversible storage of 5.6 wt% can be achieved for $NaAlH_4$. However, the kinetics of these complex hydrides was still very slow. Newest results showed that using nanocrystalline materials in combination with titanium nanoclusters consisting of only 13 atoms can drastically improve the reaction kinetics with hydrogen and lower the release temperature even further. This opens new hopes to find complex hydrides with suitable reaction kinetics by nanoscale composite compounds.

Metal hydrides are compounds formed between hydrogen and metals, alloys and intermetallic compounds. A large number of pure elements form metal hydrides, some form very stable hydrides (hardly decomposed), others form unstable hydrides (formed under very high hydrogen pressure). Reversible metal hydrides, able to give rise, for example, to storage applications, may be obtained by the association of different metals and hydrogen. Depending on whether or not an intermetallic compound is formed at the same metal composition after hydrogen desorption, the compounds are called intermetallic hydrides or complex metal hydrides.

Future of metal hydrides

The application of metal hydrides that has seen the most advanced level of development on the industrial level is the battery application (nickel-metal hydride (Ni-MH) batteries), in which hydrogen is stored electrochemically. Metal hydrides are also used for tritium storage and in niche application, like the cryo-cooling of detectors in a spatial environment.

The currently most researched application is hydrogen gas storage, related to the possible future development of a hydrogen economy. The two major advantages of the storage in metal hydrides compared to compression or liquefaction are the absence of energy loss during the storage process and the high volume capacity. The mains drawbacks are the weight capacity and the management of the thermal transfer during absorption and desorption processes.

Application	Physical phenomenon	Use
Electrochemical storage	Electrochemical formation of the hydride	Nickel-metal hydride batteries
Gas storage	Gas-solid formation of the hydride	Fuel cell supply in static or automotive applications, safe tritium storage for nuclear application
Hydrogen purification	Absorption and desorption of the only hydrogen	Hydride beds/membranes to deliver ultrapure hydrogen
Isotope separation	Different thermodynamic properties depending on the isotope	Nuclear industry, separation of deuterium from natural hydrogen
Cryo-cooler	Cooling to adiabatic expansion	Cooling of detectors in space application
Heat pumps	Storage of the heat of reaction	Heat storage for domestic use
Hydrogen gettering	Absorption of hydrogen at very low pressure	Very high vacuum

Table 3.3.1: Applications of metal hydrides.

METAL HYDRIDES		
State of the art	**Advanced synchrotron radiation and neutrons**	**Breakthrough areas**
Ni-MH batteries Hydrogen gas storage	Characterisation of the crystal structure of intermetallic compounds and metal matrix of hydrides, hydrogen localisation, study of defects, hydrogen localisation Dynamics of hydrogen diffusion Topology of hydride precipitate In-situ real-time characterisation in simulated service environments (pressure, vacuum, heat)	Novel metal hydride batteries Fuel cell supply in static or automotive applications, safe tritium storage for nuclear application Hydride beds/membranes to deliver ultra-pure hydrogen nuclear industry, safe separation of deuterium from natural hydrogencooling of detectors in space application Heat storage for domestic use

Table 3.3.2: Use of neutron and synchrotron facilities for the study of metal hydrides.

METAL HYDRIDES FOR HYDROGEN IN AEROSPACE AND AUTOMOTIVE

Potential of light metal hydrides: metal hydrides offer a safe solution for H_2-storage in mobile applications due to the extraordinary ratio of stored energy to specific weight (capacity). They would probably give a decisive push to a world based on hydrogen energy for mobile applications. Success of light metal hydrides depends on overcoming the limitations of reaction kinetics.

- Presently, sluggish reaction kinetics for absorption and desorption of light metal-hydrides limit the loading times at fuel stations, the actual availability of the necessary volumes during application, and the temperature range feasible for customer safety and wellness. The most promising route to overcome these deficiencies is the development of suitable nanocrystalline composites (Mg-hydride and metal oxide catalysts).

The solution of this challenge requires neutron and synchrotron experiments on the size and phase distribution of nanosized Mg-hydride particles and oxide catalysts. Further progress in surface and catalyst design requires time-resolved information on catalytic action obtained by synchrotron tomography experiments.

METAL HYDRIDES			
Neutrons	· Crystal structure · Hydrogen localisation · Size and phase distribution · Crystal structure of intermetallic compounds	· Dynamics of hydrogen diffusion	· Topology of hydride-precipitate
Synchrotron radiation	· Metal framework of hydrides · Study of defects · Size and phase distribution		

Fig. 3.3.11: Roadmap for research on metal hydrides.

The hydrogen storage capacity, the number of times the storage can be done reversibly, and the kinetics of hydrogen absorption/desorption are intimately linked to the alloy microstructure. Powder particles exhibiting nanostructured features have some definite advantages.

Less investigated possible applications can be found in hydrogen purification, detection or guttering, hydrogenation catalysis, isotope separation.

Importance of neutron and synchrotron radiation for metal hydrides

Large-scale facilities have always been extensively used for the study of metal hydrides. Neutron facilities are obviously necessary since neutrons are the only probe able to give information about the hydrogen atom. Both static (hydrogen localisation in crystal structure by diffraction), dynamic (hydrogen diffusion by inelastic and quasi-elastic diffusion) and topological (hydride precipitate shape by small angle neutron scattering) information may be obtained, in each case with the possibility of performing in-situ experiments of hydride formation/decomposition. Synchrotron radiation may be used in the same way with the advantage of probing smaller samples and phenomena, and with a generally better resolution and intensity. This allows studies of the defects created by hydrogen insertion and in-situ study of fast reactions.

Large-scale facilities have always been extensively used for the study of metal hydrides. Both static, dynamic and topological information may be obtained; in each case, with the possibility of performing in-situ experiments of hydride formation and decomposition.

3.3.3. CERAMIC MATERIALS

The main goal is to produce defect-free single and mixed phase ceramics with ≤ 50 nm grain size. This imposes requirements on improved process control in order to achieve reproducible and reliable behaviour during the application either of existing or upcoming materials, particularly those with a specific nanostructural design (see Fig. 3.3.12).

Nanopowder processing

Currently, there is great interest in the processing of nanopowders to make hard components. In principle, these could offer a steep jump in structural performance if nanostructured ceramics could be manufactured. The key to high performance is the ability to maintain the fine grain size of the powder in the final product and to effectively consolidate by sintering to remove defects (see Fig. 3.3.13). These two requirements place opposing demands on the sintering parameters: a high temperature provides good densification but promotes grain growth, while a low temperature limits grain growth but gives rise to retained defects. The new routes for the processing of nanoceramics, the candidate processing schemes and potential problems are shown in Fig. 3.3.14.

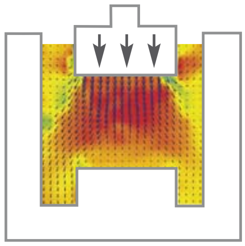

Fig. 3.3.13: Figure showing density distribution during pressure-assisted sintering.

By fast high resolution x-ray tomography, the compaction process should be tracked in real-time, helping to avoid excessive grain growth and maintaining a nanoscale structure.

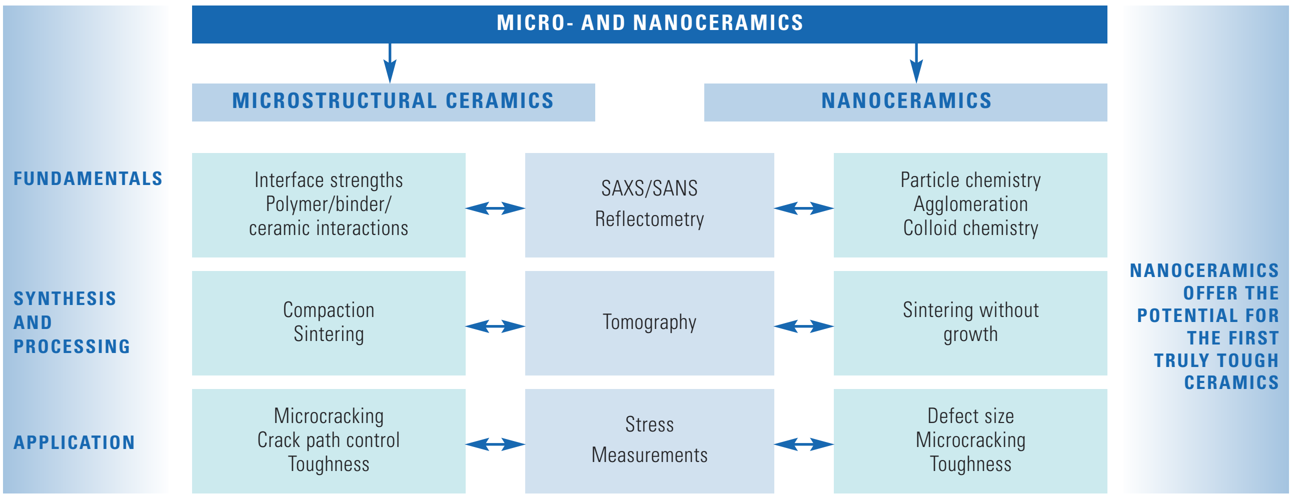

Fig. 3.3.12: Schematic roadmap for nanoceramics research.

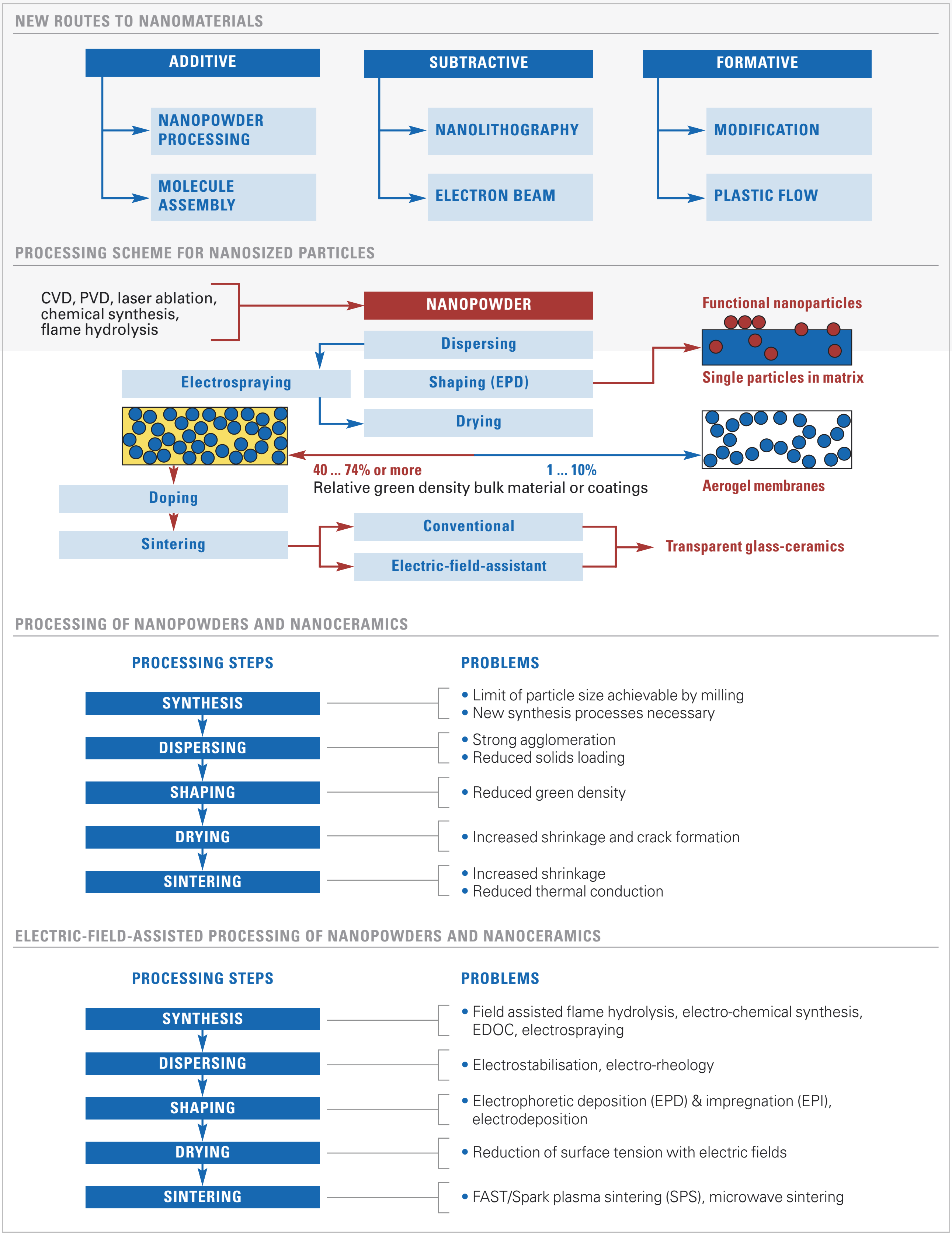

Fig. 3.3.14: New routes to nanoceramics.

Micromechanics of nanoceramics

Poor structural performance has dogged the widespread introduction of structural ceramic parts. Improved component reliability and toughness lie in finer microstructures and the elimination of defects. One approach towards designing tougher ceramics is via biomimetics, to mimic the mechanisms used by mother nature in, for instance, growth of abalone and sea shells.

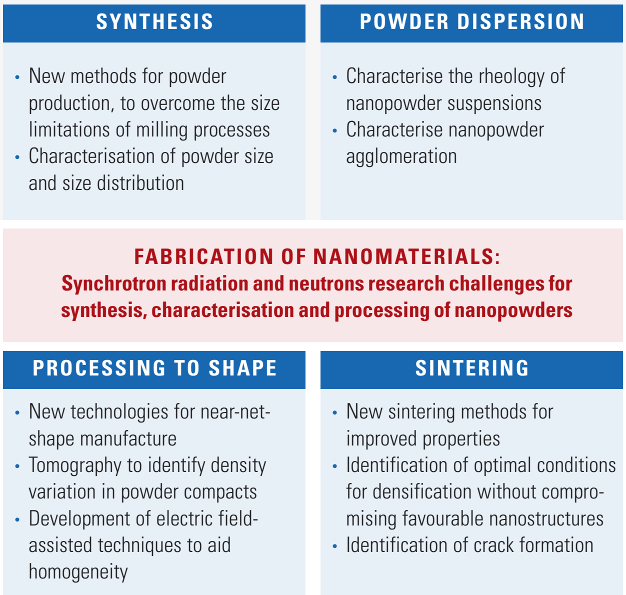

Fig. 3.3.15: Application of neutron and synchrotron x-ray methods to the characterisation of nanopowders.

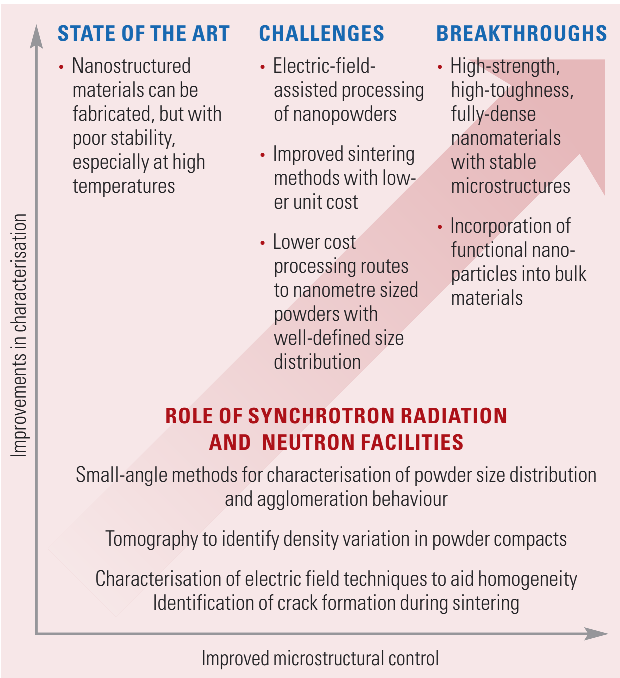

Fig. 3.3.16: Roadmap in the area of nanopowders and nanoceramics.

Attention to the monitoring of damage tolerance by structurally-designed micro- and nanomechanical mechanisms: microcracking, crack bridging and phase transformations; requires of nanotomography, space- and phase-resolved stress analysis.

The potential advances from the use of neutron and synchrotron x-rays for the study of nanoceramics and nanopowders are shown in Fig. 3.3.15 and Fig. 3.3.16.

3.3.4. COATINGS

New nanostructured coatings offer improvements in all areas of application for coating technologies, as well as offering new applications that have not been possible previously (see Fig. 3.3.17 and Fig. 3.3.18). Paints and coatings based on deposition from nanopowders can have better surface finish and durability than is currently available. Porous coatings based on nanostructured catalysts will give improvements because of their very high surface areas.

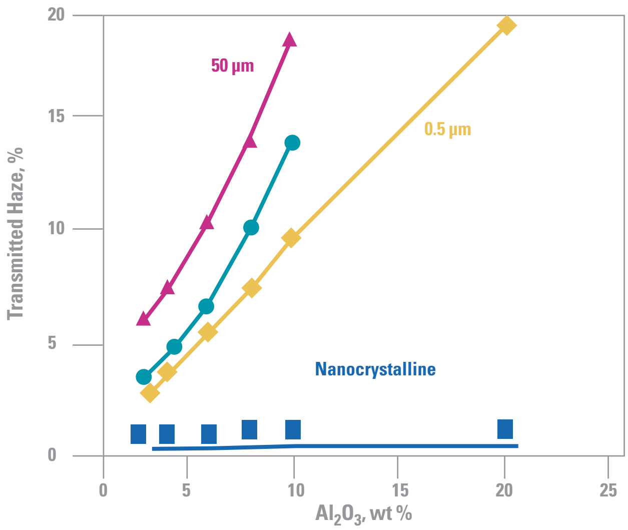

Fig. 3.3.17: Figure showing that transmitted haze drops to near-zero, if a nanocrystalline structure can be engineered.

New deposition technologies will allow for the production of coatings that are 'smart', or have embedded active electronic devices incorporated into the coatings at the time of manufacture. In order for such new applications to be developed and successfully brought to market, a range of characterisation tools will be needed, in particular neutron and synchrotron x-ray methods for the study of the surface properties, crystallography, and structure of the coated systems (see Fig. 3.3.19).

Only hard nanoceramic coatings offer sufficient transparency.

- **Abrasion resistant paints** nanocrystalline alumina offers abrasion resistance with outstanding transparency.

Advanced diffraction schemes have to be employed to measure the particle size of nanocrystalline coatings.

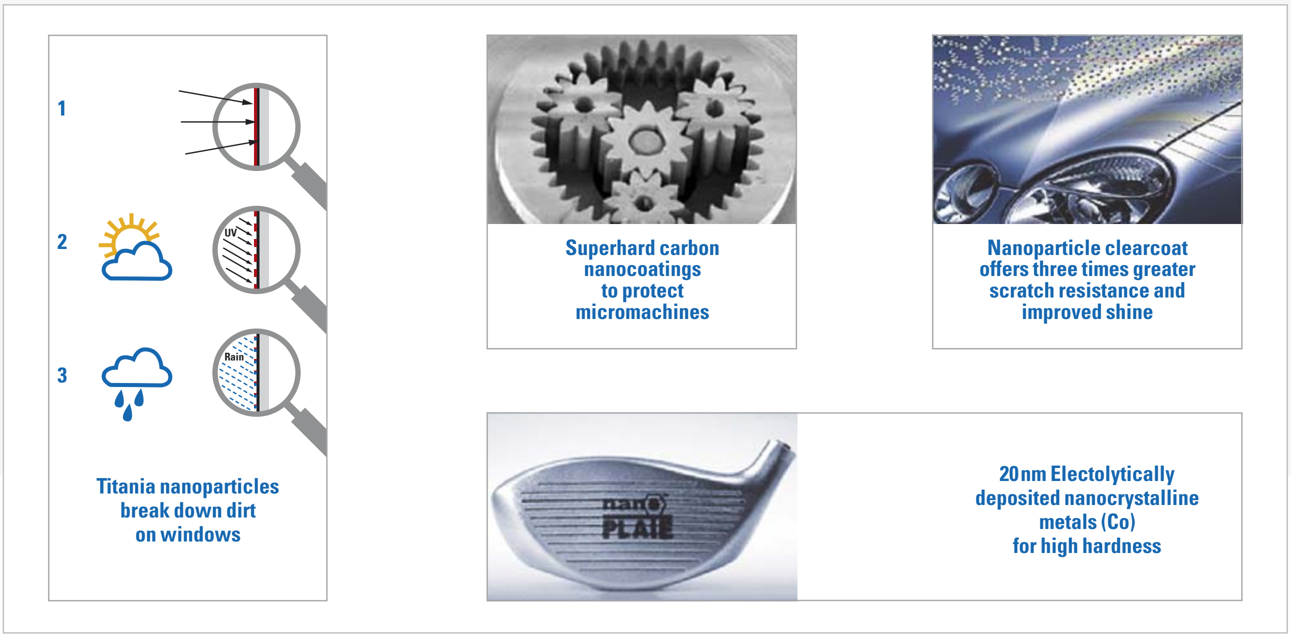

Fig. 3.3.18: Nanocoating applications.

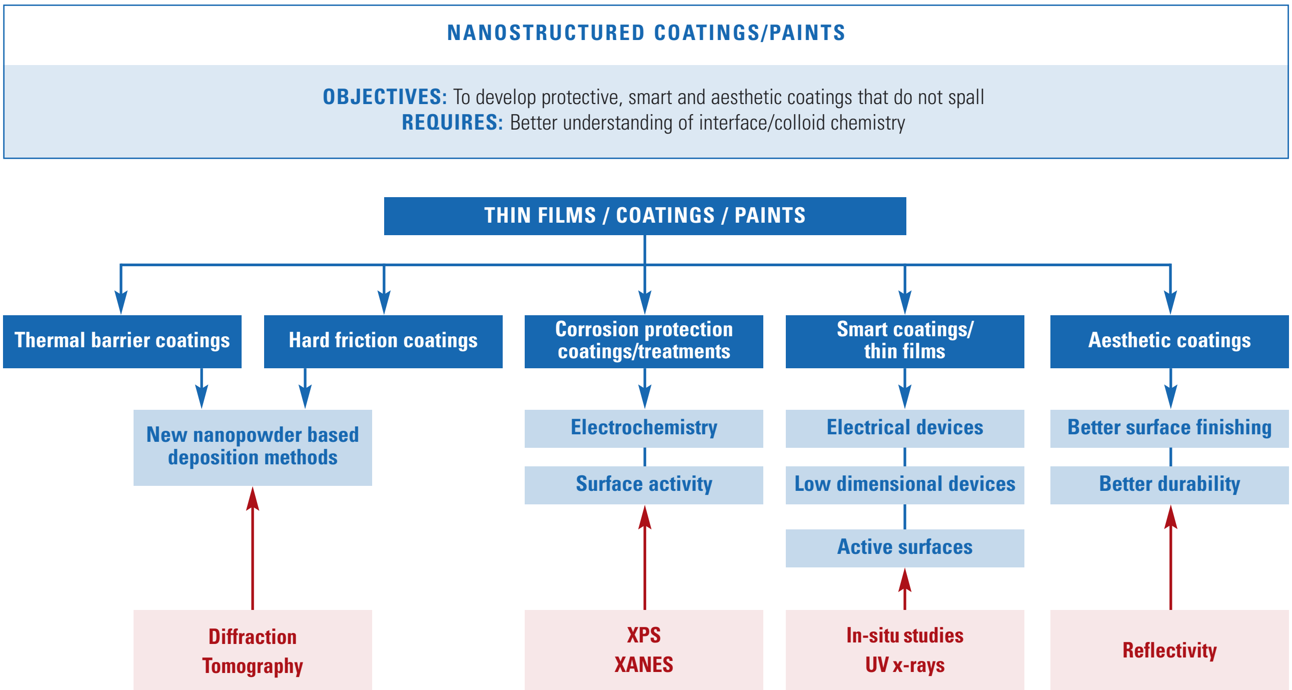

Fig. 3.3.19: Neutron and synchrotron radiation needs for nanocoatings.

3.3.5. COMPOSITES

The main objectives are:

- To develop novel process routes to deliver specific nanostructured blend and co-polymer morphologies.
- To retain nanostructure, distribution and orientation of reinforcements for improved composite properties.

An overall picture of the impact of nanostructured polymeric materials, composites and fibres is given below (see Fig. 3.3.20).

Structural polymers

Their performance is heavily dependent on the level of molecular arrangement, which can be best studied by synchrotron radiation techniques.

Polymer composites

A better understanding of impact damage is critical for the increased application of this class of material. X-ray tomography can provide information about the development of damage under a combination of impact and subsequent fatigue loading.

Polymer nanoclay systems

(see Fig. 3.3.21)

Organoclays such as montmorillonite can change the properties of composite materials drastically; for example, nylon-montmorillonite has tensile strength of up to 40% higher, tensile modulus (elasticity) up to 68% higher, distortion temperature up from 65°C to 152 °C, as well as improved flame retardant properties. The crucial dispersion and exfoliation of the clay can be studied using SAXS.

Structural fibres for composites

The C-C bond/backbone offers the possibility of very high performance (structural) fibres from a strength-to-weight viewpoint. There are various methods in use, including liquid crystalline methods (e.g. Kevlar) and polymer drawing techniques (polyethylene, spider's silk). Spider's silk has excellent elasticity and strength due to the molecular orientation as the spider spinneret draws the silk. Examination of these properties requires a microfocal beam and high flux so as to view a single fibre.

The Phonak team bike

This bike uses a frame containing carbon nanotubes. The frame weighs less than 1 kg and has excellent stiffness and strength.

Fig. 3.3.22: Phonak team bike.

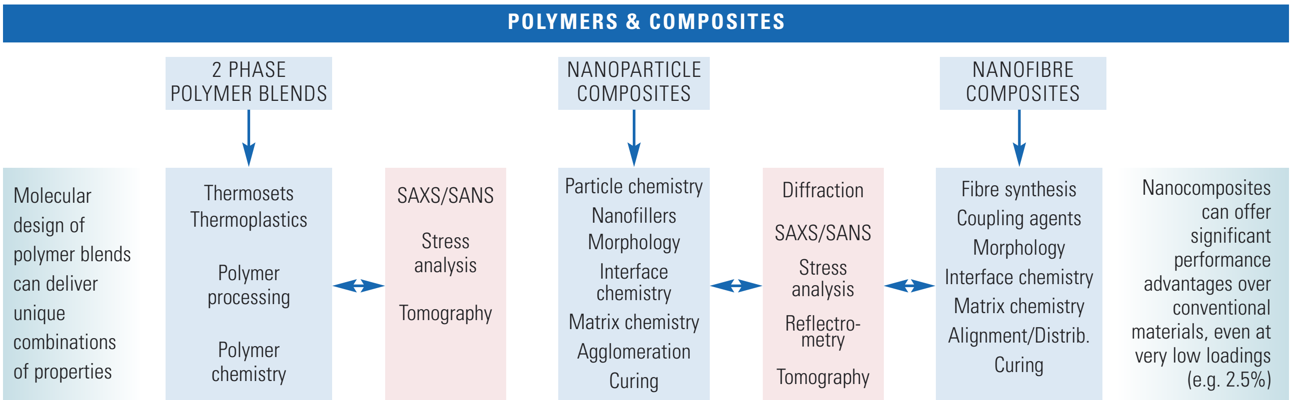

Fig. 3.3.20: The potential impact of nanotechnology to polymer-based materials, and the need for neutron and synchrotron methods for achieving key research goals.

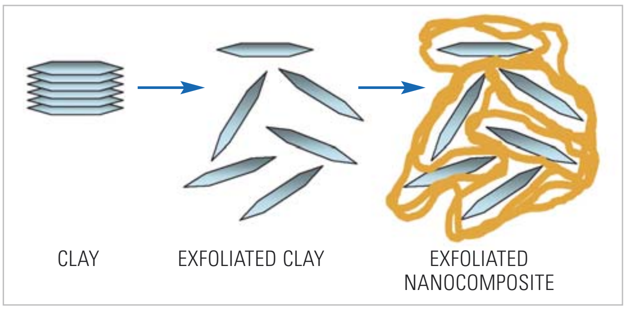

Fig. 3.3.21: Use of conventional clays for the fabrication of nanocomposites.

Self-healing nanocomposites

The incorporation of microcapsules, which, on the passage of a crack, break open. The healing agent in the capsules acts as a catalyst, triggering polymerisation, thereby leading to the closing of the crack faces.

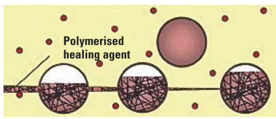

Fig. 3.3.23: Use of a self-healing phase for crack healing in nanocomposites.

Synchrotron techniques provide unparalleled detail on the nanoscale and thereby accelerate and enlighten the development cycle for new materials. Furthermore, some structures can only be understood with the help of neutron and synchrotron radiation techniques. In many cases, these techniques will offer unique possibilities for the non-destructive analyses of nanomaterials and nanocomponents.

This offers the possibility of studying the rapid evolution of micro-structure in-situ either during processing or subsequently in service.

Spectroscopy, small angle scattering and diffraction methods allow the spatially resolved determination of gradients in the atomic structure, chemical composition and microstructural inhomogeneity in nanomaterials.

Diffraction, small angle scattering, spectroscopy and possibly also tomography allow for the characterisation of microstructure changes of nanomaterials during handling and converting them into engineering components.

Fig. 3.3.22: Use of nanomaterials.

3.3.6 NANOMINERALOGY

Economy and industry uses natural minerals as merchandise on a mass scale, in the clay and cement industry, or in jewelry. Specific interest lies in minerals which show a strong potential for application in materials science related fields; among these, layer silicates are very prominent. Millions of tons are processed and traded worldwide each year.

Natural nanosized minerals show interesting structure-functionality relationships which can be manipulated on a wide range, or are already present in different varieties occuring in natural deposits. Nanomineralogy focuses on the tailored improvement of these materials for new products. Naturally occuring nanominerals can replace synthetic materials, thereby facilitating a sustainable future.

- **Vision:**
  - Establishment of a low cost nanotechnology by capitalising on natural occuring nanoparticles, which are available as mass raw materials.
  - The scientific vision encompasses the full structural and functional characterisation of the nanoparticle clay system by a set of analytical tools preferentially assembled at a single workplace.
  - Impact of the detailed structure-function relationship on processing and on the quality of present and new products.

- **Mission:**
  - This approach demands the production/manipulation of functionalised nanoparticles as mass materials (tons) on the nanoscale emerging from a fundamental understanding of the structure (including surfaces) and properties of nanominerals.
  - Highly brilliant synchrotron radiation and neutrons will be an essential element in this mission.

Clay minerals are the base for a wide span of applications, e.g. nanocomposites with tailored chemical and magnetic properties for filters in nanobiotechnology. In polymer clay nanocomposites (PCN), a few wt.-% of each silicate layer of clay mineral is randomly and homogeneously dispersed on a molecular level in the polymer matrix. When moulded, the mechanical, thermal and barrier properties of these materials are superior to those of pristine polymers and/or conventional composites. It has been shown that molecular sieves of type Si/Al-MCM-41 can be successfully synthesised by applying commercial clay containing Na-saturated montmorillonite.

Materials

- Natural layer silicates;
- Zeolites (including MCMs);
- Layered double hydroxides (LDH);
- Synthetic mass-tailored layered silicates or layered materials.

Properties

- High aspect ratio, 1:50 ... 1:200 with a thickness of 0.7 nm up to several nm;
- Various shapes: sheets, rods, spheres available from a few nm to µm size;

- Variety of surface groups, chemical bonds: functionality;
- Intercalation of different chemical compounds: functionality, mass tailoring of properties, e.g. refractive index;
- Pillared Clays (PILC) and magnetised PILCS (mPILC): microporous catalyst (PILC) with magnetic properties for purification application based on magnetic separation technology.

Applications

- Nanocomposite: stress-strain improvement, conductivity, transparency;
- Pigments: color effects, color stabilisation, surface structuring;
- Ceramics: improved properties, cost reduction e.g. during processing;
- Food design: new or advanced functionality;
- Biotechnology: application in magnetic separation technology.

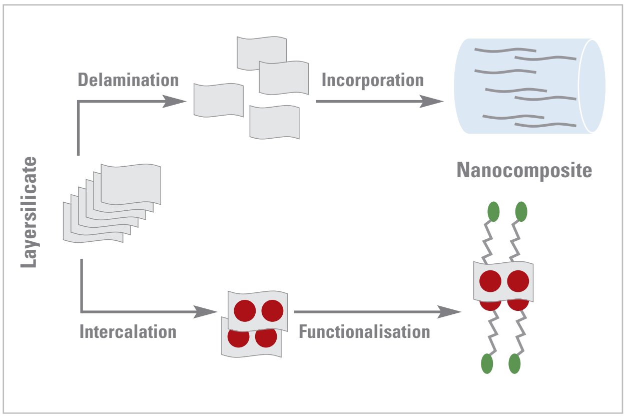

Fig. 3.3.23: Composite formation and functionalisation on layer-silicates.

Research challenges

The potential of layer-silicates lies in the high aspect ratio, high specific surface area, and the surface groups for chemical and physical (e.g. magnetic) modifications. Fig. 3.3.23 shows the potential for the synthesis of nanocomposites materials and for materials functionalisation. The interlayer region in which a variety of chemical compounds can be intercalated provides the possibility for the incorporation into other matrices and as such improving the properties of the composite. This requires an understanding on the molecular scale in order to provide the base for a technology bridging the nano- with the micro-scale. Fig. 3.3.24 highlights the research potential for nanomineralogy.

Layered silicates such as clays do not naturally form highly ordered structures. This variability can be used in a number of ways. For instance, ordered kaolin which is relatively inert when exposed to an alkaline solution can be made very reactive by heating at elevated temperatures (dehydroxylation), where crystal disorder occurs. This control of the nanostructure enables new materials such as geopolymers to be manufactured. Geopolymers are interesting in their own right but can also be used as a precursor for the production of high performance ceramics such as pollucite and leucite.

Future role of synchrotron radiation and neutron facilities

Fig. 3.3.25 shows a research roadmap of the contribution of synchrotron radiation and neutrons on the improvement of the functionality and complexity of clay particles systems.

The rapid development of synchrotron techniques has greatly expanded the range of measurements that can be undertaken and thus the level of characterisation that can be achieved. The availability of highly brilliant sources have ensured that in-situ experiments reveal-

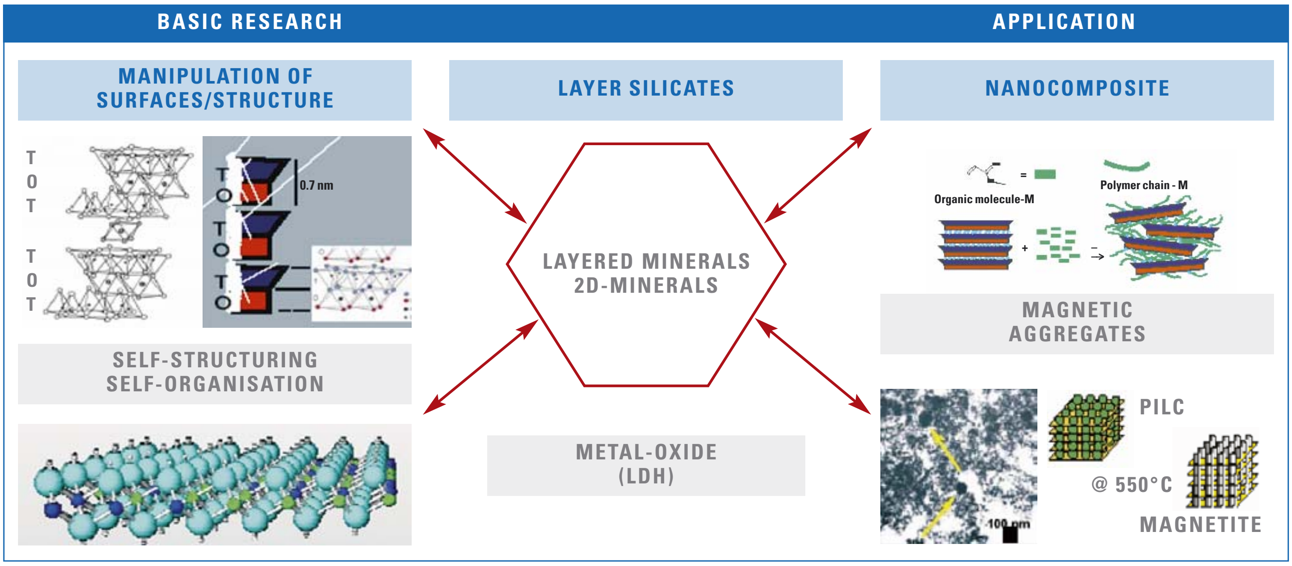

Fig. 3.3.24: Mineral research resulting into new nanomaterials.

ing changes in structure with variation of temperature, pressure and chemistry can be readily undertaken. The combination of high Q data and evolving software has also facilitated access to structural data from poorly ordered structures through PDF analysis. It should be recognised that the expansion of synchrotron techniques has opened up, and will continue, to provide new information at an ever increasing rate at better spatial and energy resolution. An example is the ability to study the growth of monolayers under controlled conditions by in-plane and out of plane grazing incidence diffraction. This is particularly important when studying self-assembly of bio-functionalised clay systems.

The progress in synchrotron techniques has been matched by the development of neutron techniques. This is particularly important as the two techniques compliment each other. The ability to obtain near-surface (x-ray techniques) and bulk (neutron) information from the same material is one example of the complimentarity although sensitivity to low and high atomic number samples is another.

The research highlights and the role of synchrotron radiation and neutrons are shown in Table 3.3.3.

The following observations appear important:

- Synchrotron radiation provides spatial resolution with the necessary intensity to study crystals in the <10 µm range. Dedicated beam lines for nanodiffraction/spectroscopy which can measure at the same spot sequentially without removing the sample are necessary;
- Improvement of focusing systems is needed for increase in spatial resolution;
- More requests for magnetic neutron scattering experiments will emerge in the future;
- The establishment of a close cooperation between material sciences with organic chemistry and microbiology and bridge the gap between pure chemistry and structure related work of mineralogy.

Supporting techniques: Electron microscopy

Electron microscopy provides direct viewing of structures down to the atomic level. This powerful technique also compliments synchrotron and neutron techniques. The key to successful transmission electron microscopy (TEM) is specimen preparation but once this is achieved it becomes an essential techniques for nano- to micro-characterisation. The ability to image a structure, obtain diffraction information as well as being able to determine elemental composition simultaneously from an area with a radius of a nanometre is remarkable. Even specimen preparation is being addressed via the focused ion beam SEM (FIB-SEM) where TEM specimens can be cut and extracted from specific locations. The combination of SEM and TEM has been impressive but future developments in resolution will see true atomic resolution from aberration corrected instruments.

Conclusions and recommendations

Synchrotron radiation and neutron experiments are pre-requisites for a comprehensive understanding of the structure-property relationship of nanominerals. These in turn will lead to further development of new materials/products and improved processes.

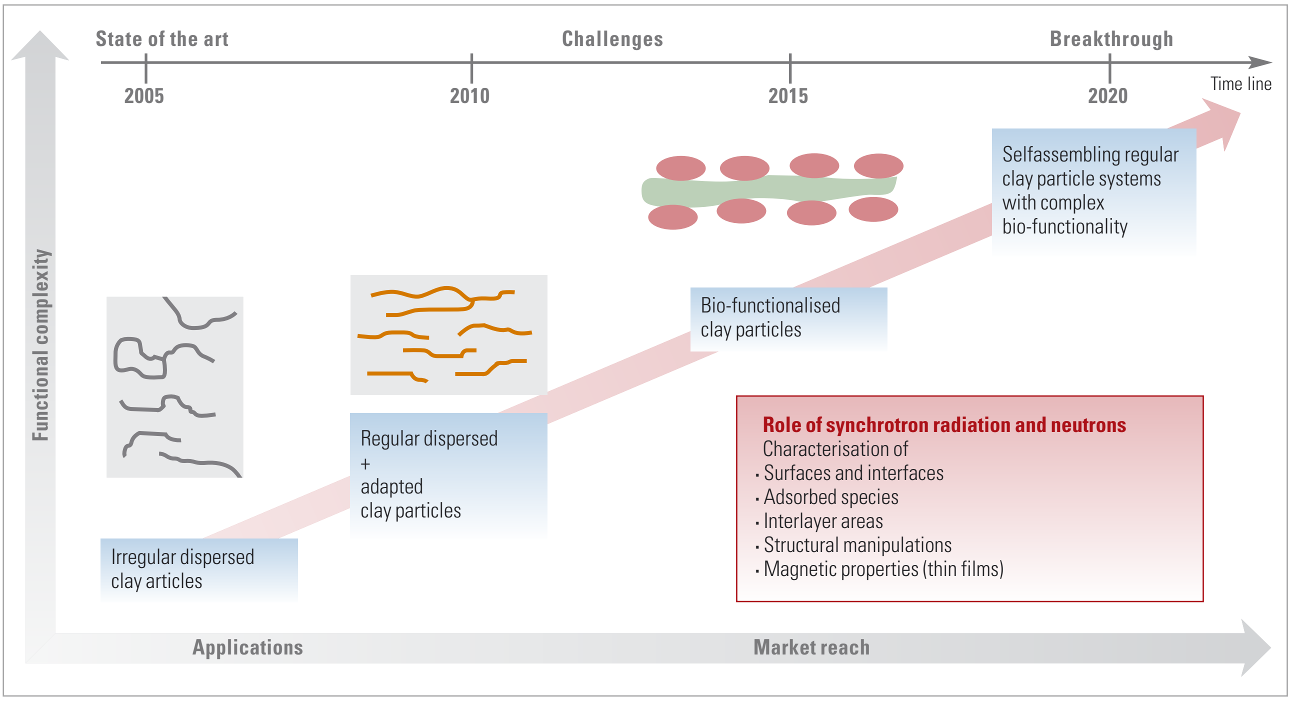

Fig. 3.3.25: Research roadmap of the contribution of synchrotron radiation and neutron on the improvement of the functionality and complexity of clay particle systems.

METHOD	KEY QUESTION	SYNCHROTRON/NEUTRON OPTIONS
Far-infrared spectroscopy (FIR)	Intercalation state, orientation of in-/organic molecules in the interlayer space of layer silicates	Only synchrotron-based FIR allows the spatial resolution and provides the intensity needed
Infrared spectroscopy (FT-IR)	Spatial resolution of binding behaviour between nanoparticle and polymer matrix	Only synchrotron-based FT-IR allows the spatial resolution and provides the intensity needed
Small/Wide angle x-ray and neutron scattering	Delamination state of layer silicates, full or partial, important for subsequent examination of disper-sion degree in polymer matrix	Spatial resolution will push the use of synchrotron radiation
X-ray diffraction (XRD)	Structure of layer silicate based on single crystal diffraction	Synchrotron radiation provides spatial resolution and intensity in order to study crystals in the <10 µm range
Powder x-ray diffraction	Structure analysis where preparation of suitably sized single crystals is not possible	Structure analysis via full pattern refinement. Crystallite size, strain and dislocation density are also extractible
X-ray absorption spectroscopy (EXAFS)	Binding strength of low mass elements especially C, P, Si to the surface of clay particles	Synchrotron radiation provides some information only for very high concentrations – this depends on the mode of operation (transmission or XRF). Good sensitivity is possible. Need for the improv-ment of detection limits indispensable
Magnetic neutron scattering	Magnetisation of clays leads to magnetic thin films, which are difficult to analyse with conventional means	Neutron scattering provides an extensive tool-box to tackle the comprehensive characterisation of bulk and magnetic properties
Reflectometry and grazing incidence diffraction	Evolution of self-assembly of bio-functionalised clay systems	Both synchrotron and neutron techniques can contribute here
Micro-fluorescence and diffraction	Monitoring binding of specific elements bound to clay – sensitive quantitative analysis will be required	Synchrotron radiation will be the only possibility

Table 3.3.3: Overview of synchrotron radiation and neutrons impact in nanomineralogy

3.3.7. NANODIAMOND

Diamond generally has outstanding materials properties: high mechanical and chemical stability in combination with its high thermal conductivity and a low friction coefficient makes diamond an attractive material for many applications. The broader application of diamond is still hampered by the cost of the material, limited geometries that can be achieved by mechanical grinding or sintering of powder particles and the lack of alternative structuring methods.

Novel CVD-processes for diamond growth are being developed, resulting in the reliable fabrication of polycrystalline and fine-grained diamond films and layers of extraordinary mechanical strength. Recent progress in plasma structuring of diamond films in analogy to silicon technology basically allows the fabrication of diamond parts with a complex and intricate shape. Low-grade CVD diamond layers with a polycrystalline structure and large cellular grains contain a large number of defects and exhibit a surface roughness that prevents the application of these new technologies.

The growth of nanocrystalline diamond layers with a grain size and comparable surface roughness of less than 10 nm is desirable. These ultra-smooth and low-stress nanodiamond layers with a thickness of up to 100 microns could be grown on single-crystal silicon wafers or other appropriate substrates by a hot-filament CVD process in a controlled atmosphere. Microparts could be produced from nanodiamond using photolithography methods already established for silicon microtechnology. This should allow the fabrication of complex shapes at a lateral resolution better than 0.5 µm. In addition, the reactive plasma etching technique (RIE) can be further implemented to chemically modify the surface within the range of a few nanometres by oxygen, hydrogen, fluorine and other elements.

Highlights for research

The high mechanical stability and strength in combination with the low coefficient of thermal expansion, high thermal conductivity, low coefficient of friction, excellent wear resistance, chemical inertness and outstanding biocompatibility make nanodiamond an attractive material for many applications in the field of microsystems: i.e. micro-actuators, heat spreaders, lenses and laser windows, electronic devices such as diodes and transistors, MEMS, cutting tools, surgical tools, biomimetic surfaces, etc.

In order to achieve a reliable production technique, future research in this field should focus on the:

- Advancement of reliable synthesis methods;
- Up-scale of synthesis;
- Theory of controlled crystal growth;
- Equiaxed nanostructures and ultra-smooth surfaces;
- Geometric accuracy achieved during the reactive ion etching (RIE) process;
- Chemical composition and surface termination;
- Preparation of biomimetic surfaces.

Scientific and industrial breakthroughs can be expected for: (i) microparts and micromachining, (ii) cutting tools and (iii) bio- (mimetic) surfaces (see Fig. 3.3.26).

• Microparts

The reliable production and use of microparts is currently limited to the use of silicon as a structural material. Silicon can be processed and shaped by a number of established methods, but, unfortunately has very limited mechanical reliability due to its inherent brittleness. The alternative use of nanodiamond can overcome these limitations as a bulk material or even as an ultra-hard coating.

As such, the aim of research is to improve the basic understanding and establish reliable production methods that can overcome the following problems:

- Fracture or chipping of microcomponents by manipulation or shock;
- Destructive wear on mechanically stressed components;
- Assembly problems;
- Modification of surfaces through friction and wear;
- Peripheral problems e.g. damage by washing/cleaning of parts.

• Cutting tools

The radius of curvature of the cutting edge of any cutting tool is the key parameter in this context. For different applications, industrial or medical, this diameter can be varied through the plasma etching process of nanodiamond between a few nanometres (free standing blades) and 1 micrometre (nanodiamond coatings). As such, the most important goal is the increase of the lifetime of cutting tools by a factor >10 in comparison with conventional WC-Co, TiN and other ceramics.

• Nanobiology – nanomedicine

There are presently several fields in which new materials with biocompatible surface properties are urgently needed: Stem cell research (desperate need for new materials with niche-like structures), conventional biomedical engineering (need for advanced biomaterials whose biocompatibility is precisely adjustable) and research focusing on biodurable materials with structures inhibiting or enhancing bacterial or cell growth. The goal here is to mimic the native environment of a certain biological cell through microetching and to control the surface termination chemically.

For example, Fig. 3.3.27 shows an example how a biological surface – a strawberry – can be transferred into a nanodiamond surface structure.

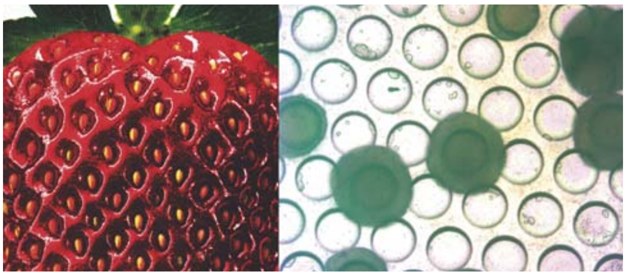

Fig. 3.3.27: Surface of a strawberry (left) and the corresponding biomimetic surface of nanodiamond produced by RIE, together with the cultivation of established stem cells (for example P19) with embryoid bodies sticking on holes with a diameter of 200 microns (right).

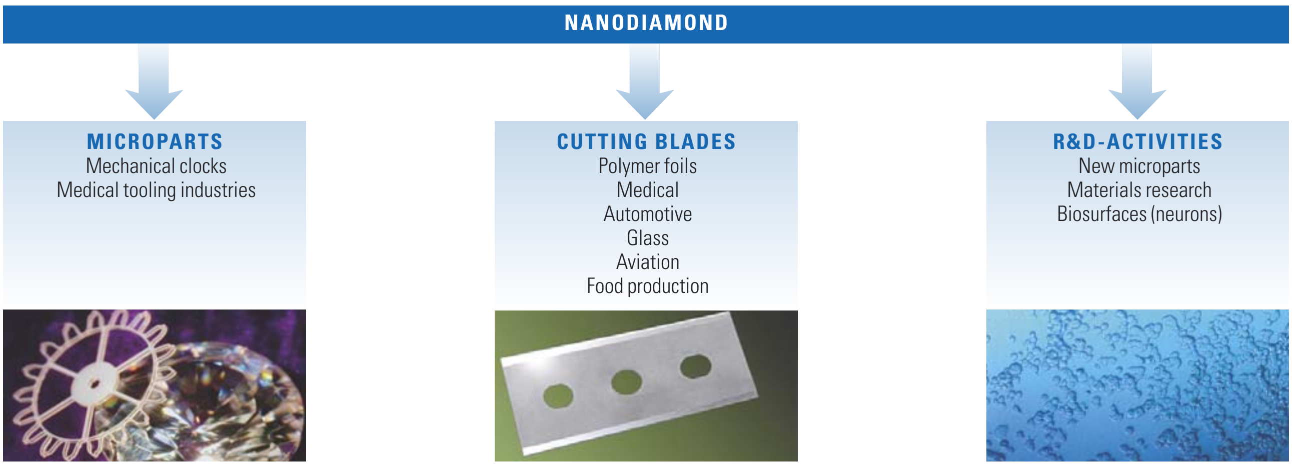

Fig. 3.3.26: Areas of applications for nanodiamond.

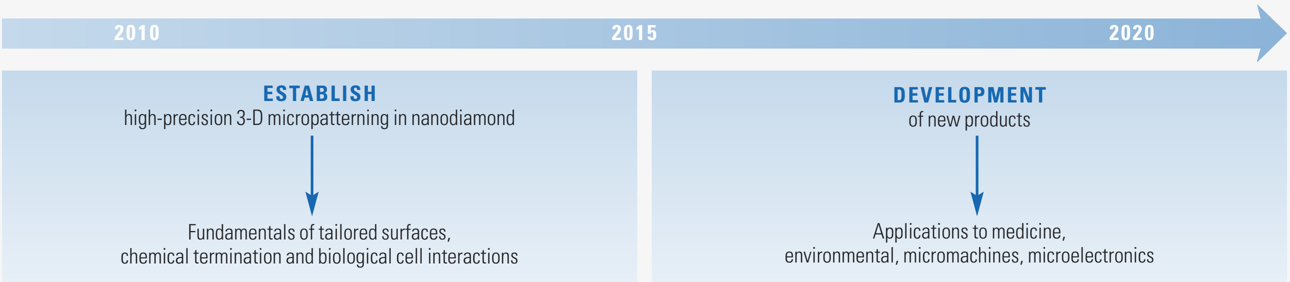

Fig. 3.3.28: Research roadmap for nanodiamond materials.

This field of research is new and will provide significant breakthroughs in the near future regarding bioreactors, biocompatible materials and lab-on-chip technologies. The main aims are to structurally modify the surface of nanodiamond in order to mimic biological structures (lotus flower, strawberry etc.) and, in addition, tune the surface chemistry in order to tailor or switch the interaction with living cells or bacteria in a unprecedentent way.

Importance of synchrotron and neutrons

- Characterisation and understanding of defects and mechanical stress in nanodiamond layers on silicon as a function of temperature;
- Characterisation of microstructure (grain and phase distribution, content of 2nd phases, temperature dependent stability, porosity and other extended defects);
- 3-D chemical elemental mapping;
- Improved patterning techniques by x-ray lithography;
- Analysis of adsorbed surface water and cell interaction under different conditions (switching by laser).

Conclusions

The European research strategy should focus on:

- New methods and products which place Europe as a forerunner in this field of research;
- Lubrication-free and wear-free components for microsystems;
- Novel applications under extreme conditions (temperature, pressure, environment);
- New concepts to increase the efficiency of bioreactors;
- Biomimetic materials;
- Tunable biological surfaces using laser light and other LED methods;
- Electronic devices and sensors in operation at high temperatures.

3.3.8. CONCLUSIONS AND RECOMMENDATIONS

Beam lines at large-scale facilities need to be adapted for the extraordinary high spatial and also angular/energy resolutions that are required. The demands on high spatial resolution for probing structural inhomogeneities in nanomaterials will necessitate nanometre-sized synchrotron radiation beams. For probing defined gauge volumes in nanodevices, adaptations of the sample handling systems and the control of the beam position are prerequisites.

The current techniques for microstructure analyses will need to be substantially adapted due to the local disorder and non-uniformity of the nanomaterials. Future impact on nanomaterial research can be expected from the even higher photon flux, higher brilliance and coherence of the synchrotron radiation at future synchrotron sources and the XFEL. The diagramme gives an overview of the needs required by structural nanomaterials scientists (see Fig. 3.3.29).

For Europe to approach the rate of development being achieved in the USA and Japan, it is essential to establish an expert 'Structural Nanomaterials Centre' with access to both neutron and synchrotron facilities as well structural and microstructural characterisation facilities. If provided under a research hotel-style environment, this could provide users from across Europe with the necessary access to a full range of in-situ facilities needed to probe behaviour at the nanoscale under service or processing conditions.

There is a wide range of opportunities across the field of structural materials that can be facilitated either by today's, or by improved, neutron and synchrotron instruments (see Fig. 3.3.31). Synchrotron radiation and neutron facilities will naturally become a focus for nanomaterials research and technology in Europe. The competitive scientific and industrial interests will push the existing infrastructure capabilities such that the challenges will need to be met (outlined in Fig. 3.3.30).

Summary guidelines

Further contributions to the development of nanomaterials demands:

- Better links between: basic research, materials characterisation, materials engineers and end users;
- Neutron and synchrotron instruments capable of studying devices and components – not just samples;

- More materials engineers with experience in neutron and synchrotron diffraction techniques;
- Greater collaboration between facilities, academics and industrial teams in designing/carrying out experiments – this would be aided by a pioneering 'Structural Nanomaterials Centre' providing leadership and unique facilities;
- Faster experiment turnaround at facilities to accelerate product development.

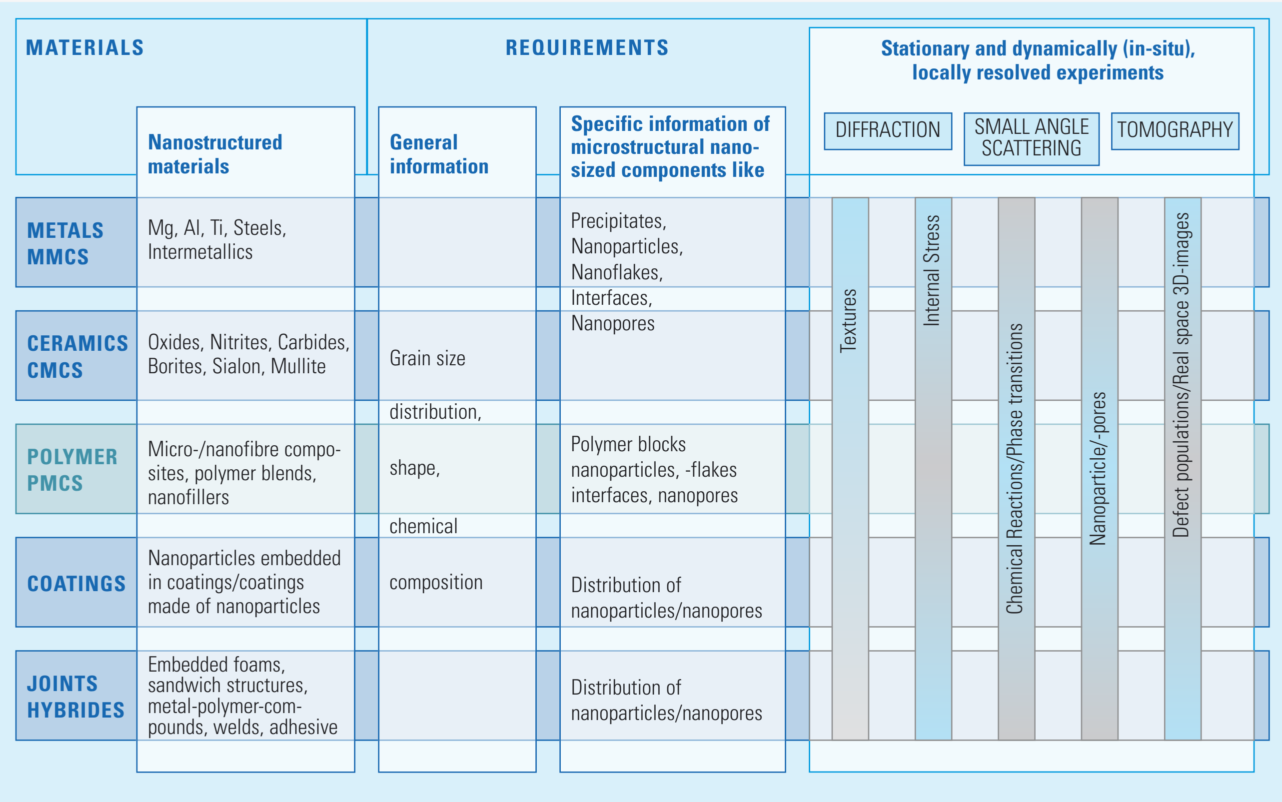

Fig. 3.3.29: Research challenges for nanomaterials and the impact of neutron and synchrotron x-ray methods.

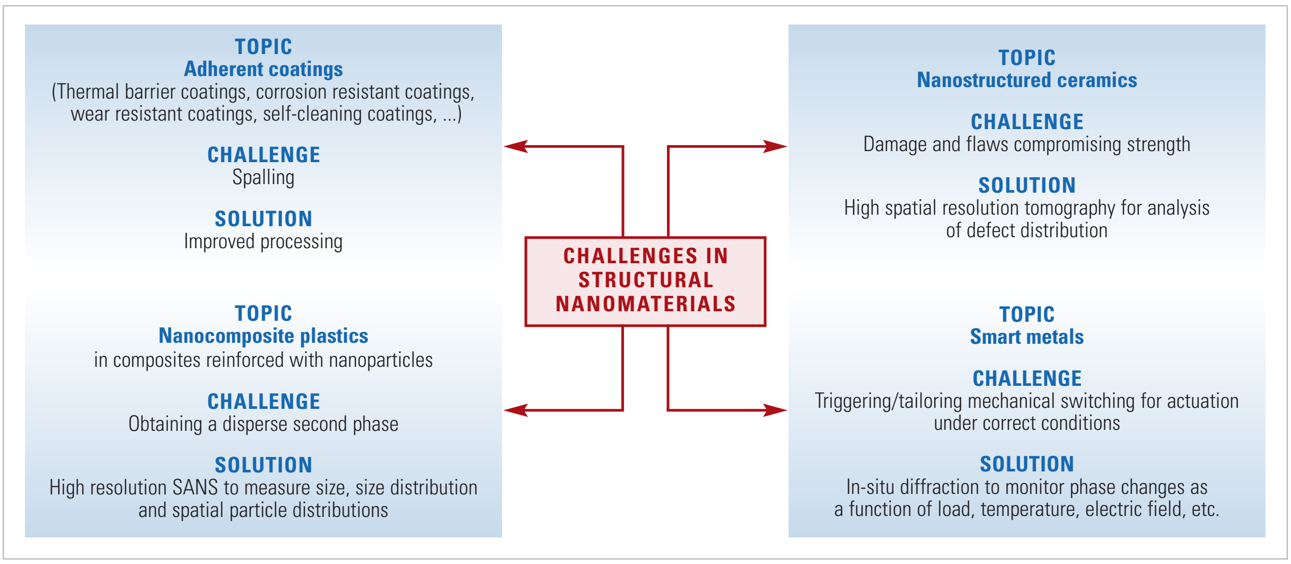

Fig. 3.3.30: Key research challenges for nanomaterials and the role of synchrotron and neutron methods.

It is recommended to set up a 'Structural Nanomaterials Centre' with good access to state of the art neutron and synchrotron facilities (see Fig. 3.3.32 and 3.3.33). Given the investment in dedicated centres for structural nanotechnologies in USA and Japan, e.g. at Oak Ridge National Labs, this effort has to be accelerated in Europe.

The 'Structural Nanotechnology Centre' would need intimate access to a varied range of neutron and synchrotron techniques with in-situ rigs to enable the assessment of structural performance under realistic in-service conditions, and in addition, access to traditional materials characterisation techniques (electron microscopy, DTA, mechanical testing equipment), as well as materials processing facilities. Key to its success will be a close relationship between materials scientists, polymer scientists, and ceramists, as well as industrial engineers involved in research and development. No such centre exists across Europe at present.

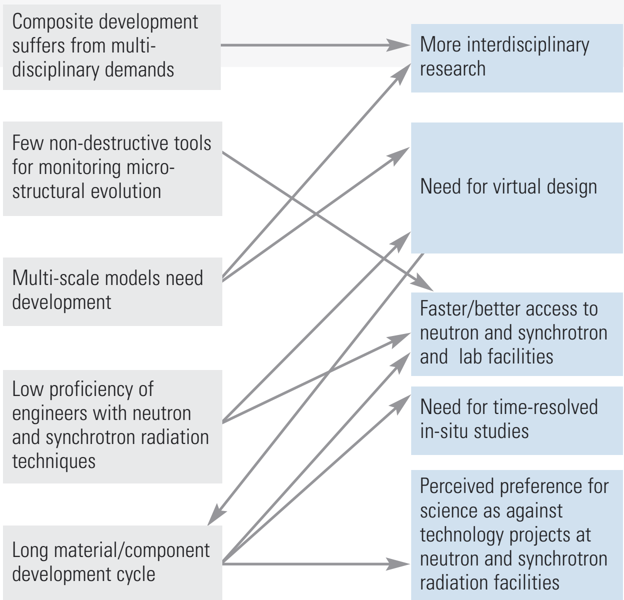

Fig. 3.3.31: Opportunities for improving the linkage between engineering and large-scale facilities.

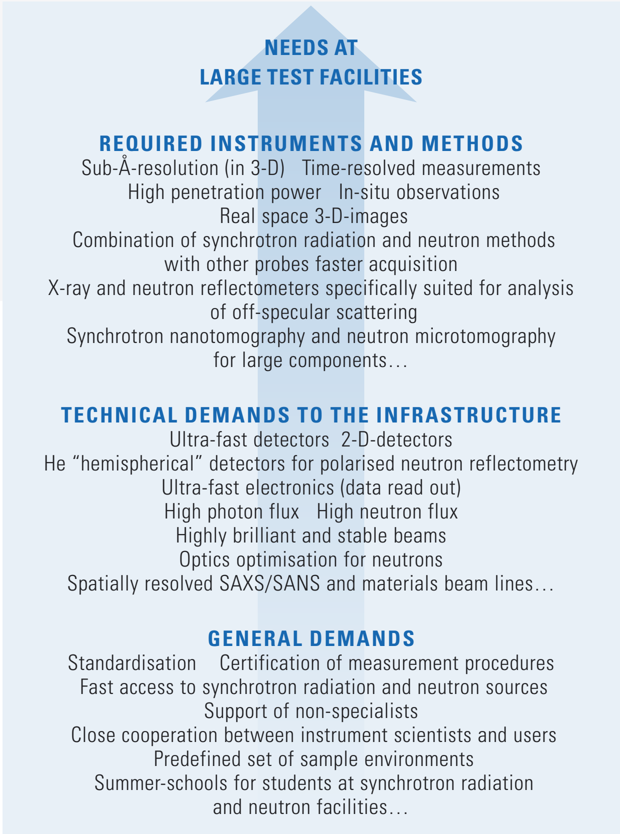

Fig. 3.3.33: The challenges for the formation of a European Structural Nanotechnology Centre.

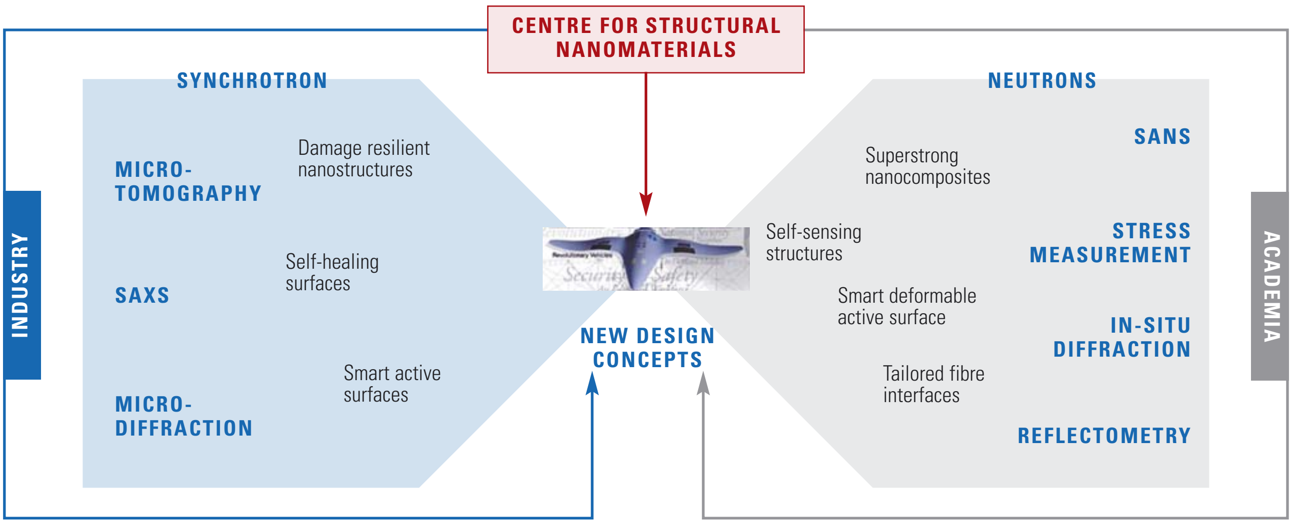

Fig. 3.3.32: A "Structural Nanotechnology Centre" would pioneer a multi-technique approach to in-situ observation of nanomaterials and devices under realistic conditions.

3.4. FUNCTIONAL NANOMATERIALS

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Functional materials are responsive to external magnetic or electric fields, to temperature, pressure or chemical potentials. Their response can be used as a sensor or as an actuator.

Functional materials include all types of chemicals, ranging from organic to inorganic, from metallic to covalent, and from molecular to macromolecular species. In devices, the useful form may be a single crystal, a compound, a thin film or a composite. At the basic level, this offers the possibility of the miniaturisation of a device, with gains in space saving, lower weight, improved heat dissipation, and so forth.

These smart materials are underpinning the technological developments of the 21st century, and play an increasingly important role in the economy and our daily lives, with applications ranging from the automotive, communications and consumer industry to health care. Their functionality can cover a wide range of physical properties, such as piezoelectric, magnetostrictive and semiconducting materials, as well as chemical properties, such as catalysis, absorption, chemical sensing, and electrochemical behaviour. Moreover, these smart materials can adapt, or respond to their environments (see Fig. 3.4.1).

The trend in functional materials is towards increasingly smaller dimensions. The interaction between the multiple structures in the components, with ensuing complexity, e.g. quantum dots or magnetic patterned arrays, demands novel destruction-free and in-situ analytical techniques. One of the most important analytical techniques is scattering using photons and neutrons. In the future, novel scattering techniques for the analysis of nanoscale functional materials have to be provided by the European synchrotron radiation and neutron facilities.

Furthermore, simply by reducing the size of a material to the nanometre scale, even when in only one dimension (e.g. in the realisation of an ultrathin layer) its physical properties change. This is due to quantum confinement effects modifying the electronic properties and thus all relevant materials parameters. Technical realisations which exploit this phenomenon are quantum dot lasers, magnetic (GMR) sensors and read-out heads and (since a long time) the ultra-small metal particles in a catalyst. The materials properties of these ultrasmall structures need to be explored, even on the individual basis of a single selected nanoparticle. This can be achieved by using advanced spectroscopic methods, combined with microscopy, which are only available at the most advanced synchrotron sources.

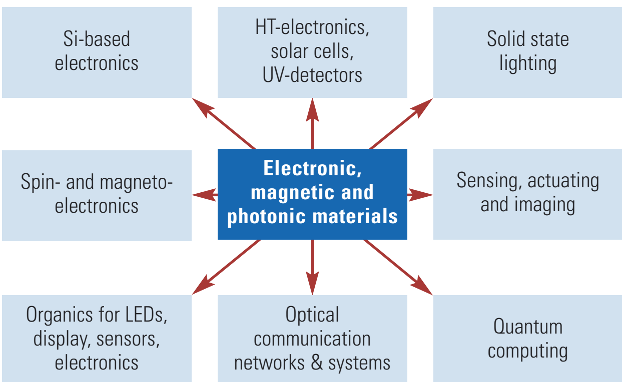

Fig. 3.4.1: Overview of functional nanomaterials.

Promising applications of nanofunctional materials

The potential uses of nanofunctional materials are:

- **Coatings:** Corrosion and wear-resistant coatings, as well as thermal barrier- and thermal gradient coatings. In future, 'intelligent coatings' will become important e.g. as a response to environmental conditions.
- **Composite materials:** Carbon nanomaterials have a range of specific electrical, mechanical and thermal properties. As an additive in polymers, ceramics, metals and textiles, these nanoadditives will improve the matrix material in terms of electrical and thermal conductivity or mechanical strength with low nanomaterial loads.
- **Energy-related materials:** A major goal is an efficient reversible hydrogen storage material. Here, novel microporous materials with an extremely high specific surface area or nanoscale complex hydrides with catalytic nanoclusters may offer the possibility to develop storage materials suitable for mobile applications.
- **Nanoelectronics:** Creation of nanoscale circuits, wires and packaging of semiconductors. The goal of industry is to use these components to manufacture a new class of very small and very powerful electronic devices.
- **Sensors:** Sensors based on nanocrystalline materials offer higher sensitivity and faster response times. These features are already being exploited in metal oxide gas sensors. However, the major problem in gas detection is in selectivity and this is not resolved in a single element sensor. Thus, the future will be in integrated nanosensors and the use of neural network methodologies for signal analysis.
- **Catalysts and fuel cells:** Carbon nanomaterials enhance the properties of fuel cells. As catalyst support material for precious metals (e.g. platinum), carbon nanomaterials can help to enhance the power density of fuel cells and help to reduce the amount of platinum.

3.4.1. ELECTRONIC AND SEMICONDUCTING MATERIALS

The impact of electronic materials on modern-day society can hardly be overestimated. Electronic technology is embedded in all branches of industry: computing, household appliances, entertainment etc. Especially in the fields of information processing and technology, the drive towards nanoscale electronics is relentless and holds the promise for increasingly smaller and faster devices. Microelectronics is generally recognised as the enabling technology for present and future information systems. However, the craving for information systems with a higher level of capacity is paving the way for the transition from microelectronics to nanoelectronics in the near future. The Semiconductor Industry Association roadmap contains SiGe buffers for strained Si layers and strained Ge from 2005 onwards and silicon

STATE-OF-THE-ART	FUTURE NEEDS AND CHALLENGES	FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRON SOURCES
Si-based electronics • Conventional Si-integrated electronics: end of improvements due to mere scaling (Moore's law) in sight (2015) • SiGe technology is well-developed in Europe, e.g. SiGe buffers for strained Si/Ge heterostructures • Europe is leading in Silicon on insulator (SOI) technology, e.g. for high-frequency devices **Si-based electronics** • New device concepts based on nanostructures developed in research, e.g. quantum dots **Optoelectronics** • Europe is behind in optoelectronics, e.g., III-V heterostructures; GaInNAs structures, II-VI HgCdTe ternary systems, ZnCdSSe and ZnSSe devices, and GaAIN for blue and UV emitters (see also the section on photonics) **Organic semiconductors** • Materials and devices developed on research level	**Future potential** • Continuous improvement of Si/SiGe technology • High-K dielectrics • Improving concepts for strained Si/Ge layers beyond virtual SiGe substrates, e.g., using quantum dots as defect-free stressors **Nanosemiconductor breakthroughs** • Organic electronic materials, e.g., for flexible displays, organic dielectrics, biosensors • Materials for powerful storage devices • New fault-tolerant computer architectures compatible to self-organisation • Spin electronics • Quantum computing materials & concepts • From nanotubes and molecular electronics to organic polymers **Fabrication challenges** • Control of growth/self-assembly • Develop reliable manufacturing processes (Combination of 'top-down' & 'bottom-up' approach) • Combination of new and existing materials and technologies • Full integration in single 'system-on-chip' components • Development of strain simulation for cross-checking experimental results **Characterisation challenges** • Organic dielectrics • Self-assembled systems • Sensitivity down to monolayers • Characterisation of nanodefects • Surfaces and interfaces • Complex alloys	**Synchrotron radiation** • Non-destructive investigation of heterostructures and buried nanostructures **Characterisation of defects, surfaces and interfaces** • Use of highly focused nanobeams (< 20 nm) for simultaneous real and reciprocal space resolution • In-situ studies during growth **In-situ studies during device operation** • Exploitation of fully coherent x-ray beams for the direct reconstruction of real space properties and to study time-correlation properties (in-situ growth, diffusion, self-organisation, degradation) • Combination of diffraction, imaging, and spectroscopy of nanostructures • Dedicated beamlines for series and failure analysis for industrial development **Neutrons** • Use well-collimated neutron beams to study the smoothness of interfaces, oxide barrier thickness, and interdiffusion with ultrahigh resolution

Fig. 3.4.2: Opportunities and challenges for synchrotron radiation and neutrons in future research for nanosemiconductors.

on insulator technology from 2003 onwards. By about 2015, these developments in conventional Si-technology will be exhausted due to fundamental physical reasons (quantum effects), as well as material properties (e.g., no reliable oxide barriers can be fabricated with the required thicknesses in the monolayer range). Therefore, alternatives are being intensively studied (see Fig. 3.4.2).

The spectrum includes thin films and superlattices, atomically corrugated surfaces, nanosized atomic clusters, assemblies of molecular materials, quantum dots and quantum wires, carbon nanotubes, and graphene (single layer graphite). The pursuit of new methods for preparation, synthesis, characterisation, and detailed examination and prediction of the properties of nanomaterials constitutes nanoscience and nanotechnology. Special technological benefits from nanoscience demand the exploitation of novel properties at the nanoscale to functionalities for industrial application. While, for instance, defects in conventional two-dimensional layers are a decisive obstacle for conventional Si technology, with self-assembled nanostructures, defect-free strained SiGe and strained Si can be fabricated. Hence, there is a clear need to control the growth of self-assembled nanostructures, and to combine this new "bottom-up" approach with the conventional lithographic structure definition ("top-down"). Apart from the challenge to create new or better materials and ever smaller structures, it might become necessary to invent new fault tolerant computer architectures, which are compatible with fluctuations in self-organised materials.

The Si-Ge technology is well-developed in Europe. In the field of optoelectronics, however, Japan and US companies are leading. This includes the development of III-V heterostructures employed in optical fibre communication systems, Ga-In-N-As structures for the production of laser diodes, II-VI Hg-Cd-Te ternary systems for very long wavelength devices, and compounds such as Zn-Cd-S-Se and Zn-S-Se and Ga-Al-N for visible and UV-light emitters.

Specific challenges for synchrotron radiation and neutron facilities

In future Si-technology, synchrotron radiation and neutron facilities must contribute to solve urgent material problems, in particular with a view to:

- The study of defects in conventional Si layers;
- The growth of defect-free strained SiGe and strained Si;
- The determination of inhomogeneous strain fields;

- The determination of inhomogeneous chemical composition profiles;
- The study of self-organised semiconductor nanostructures (quantum wires and dots).

In the development of advanced materials, several research needs have been identified:

- Use of Ge instead of Si: this transition will require extensive characterisation work, including the characterisation of the composition and the roughness at the Si interface with Ge;
- Design of foams of organic dielectrics as low-K oxides: urgent need for in-situ characterisation techniques;
- Development of Ga-N/Al-Ga-N piezomaterial: systematic destruction-free investigations of strain and dislocations;
- Tailored growth of self-assembled monolayers: systematic investigations of structure, coverage, heterogeneity and steric hindrance;
- Development of plastic electronic materials: microscopic study of the effect of grain boundaries.

3.4.2. PHOTONIC MATERIALS

One of the most important discoveries in modern optics is the fact that the optical properties of matter are not invariant but controllable. Three methods for their efficient control are known:

- Dielectric and metallic nanostructures, such as photonic crystals and microcavities.
- Composite nanostructures, metamaterials, with components whose sizes are smaller than the optical wavelength.
- Quantum confinement of electrons and holes in nanostructures, such as quantum dots, quantum wires and quantum wells.

All these technologies are achieved by the self-organisation of nanomaterials and nanofabrication.

Photonic technologies enabled high-speed broad-band telecommunication, and revolutionised displays (flat panel displays). Solid state lasers and light-emitting diodes have replaced other light sources, enabling novel optical solutions from car displays to endoscopic surgery. Compared to the US and Japan, Europe is behind in optoelectronic and photonic applications, and a large effort will be required to close this gap. Severe obstacles have to be overcome in the near future in order to further the photonic field and make it market competitive.

A similar breakthrough is expected for short-distance data exchange, e.g. between CPU's and graphics adapters or storage networks, or within local networks. Here, cost-effectiveness will be the decisive factor. So far, no light sources, modulators and detectors can be fabricated at reasonable costs and with the desired degree of integration with electronic devices. It is unclear at the moment, whether hybrid solutions (which are cost-intensive due to packaging effort) or solutions integrated on-chip will (ultimately) be the optimum solution.

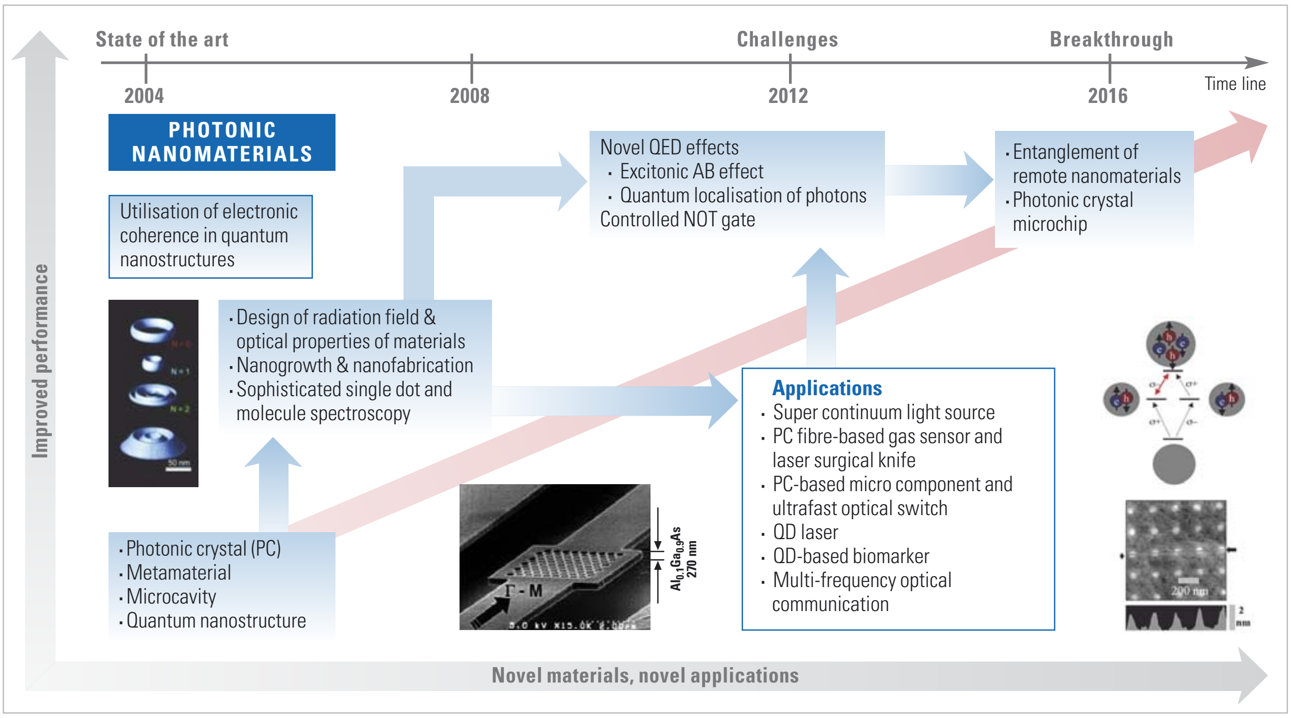

Fig. 3.4.3: Roadmap highlighting the future research on photonic nanomaterials research.

The following main fields of development can be foreseen (see also Fig. 3.4.3 and 3.4.4):

- III-V materials: GaN (405 nm) high density optical storage;
  - GaAs/AlGaAsP (660 nm) coupling to plastic optical fibres;
  - GaAs/AlGaAs/GaInP (800–1000) pumping rare earth laser;
  - InGaAsP (1310 nm) coupling to silica fibers;
  - InGaAs (1550 nm) coupling to silica fibers;
- Organic materials: highly flexible, cheap in production, low thermal budget compatible with CMOS, hybrid integration to CMOS possible;
- Integration of photonic circuits (driven by telecommunication systems). Up to 10 GBit/s hybrid integration sufficient, for >40 GBit/s monolithic devices required;
- Integration of photonic and electronic components, driven by interconnects: intra-building (also automotive and aerospace), intra-backplane (servers, eventually PCs), intra-chip.

In the search for new applications, new material developments based specifically on nanomaterials are required. In principle, two routes are followed at the basic research level: (i) the production of colloidal nanocrystals with specially designed optical properties, which have then to be incorporated in a lithographically produced device; (ii) the use of epitaxial methods and self-organisation, to directly introduce nanostructures into devices. In the latter approach, very similar prospects and hindrances are met to the ones in nanoelectronics. In turn, major challenges in material design and material characterisation, requiring novel characterisation solutions, will be encountered. These solutions will have to be developed and provided by synchrotron radiation and neutron facilities. In particular, the interface structure in heterosystems, defects, and chemical composition and strain distribution within and around nanostructures should be considered important issues (see Fig. 3.4.5).

Particular targets areas for future research exploiting synchrotron radiation and neutron facilities are (see also the following roadmaps: Fig. 3.4.3 and Fig. 3.4.4, and Fig. 3.4.5 for a schematic diagramme):

Manipulation of optical properties of nanomaterials

- Development of materials with arbitrary optical properties by sub-wavelength structures.
- Anti-reflection effect of surface nanostructures, and structural colour originating from periodic structures.
- Nanostructured optical materials ("metamaterials") with arbitrary refractive index, permittivity, or permeability.

Nanooptical circuits

- The current optical circuits based on planar waveguides are very large compared with the optical wavelength due to weak light confinement. To diminish the scale mismatch with electronic circuits and to realise electronic-photonic integrated circuits, wavelength-sized optical circuits based on photonic crystal waveguides or plasmonic waveguides is of great importance.

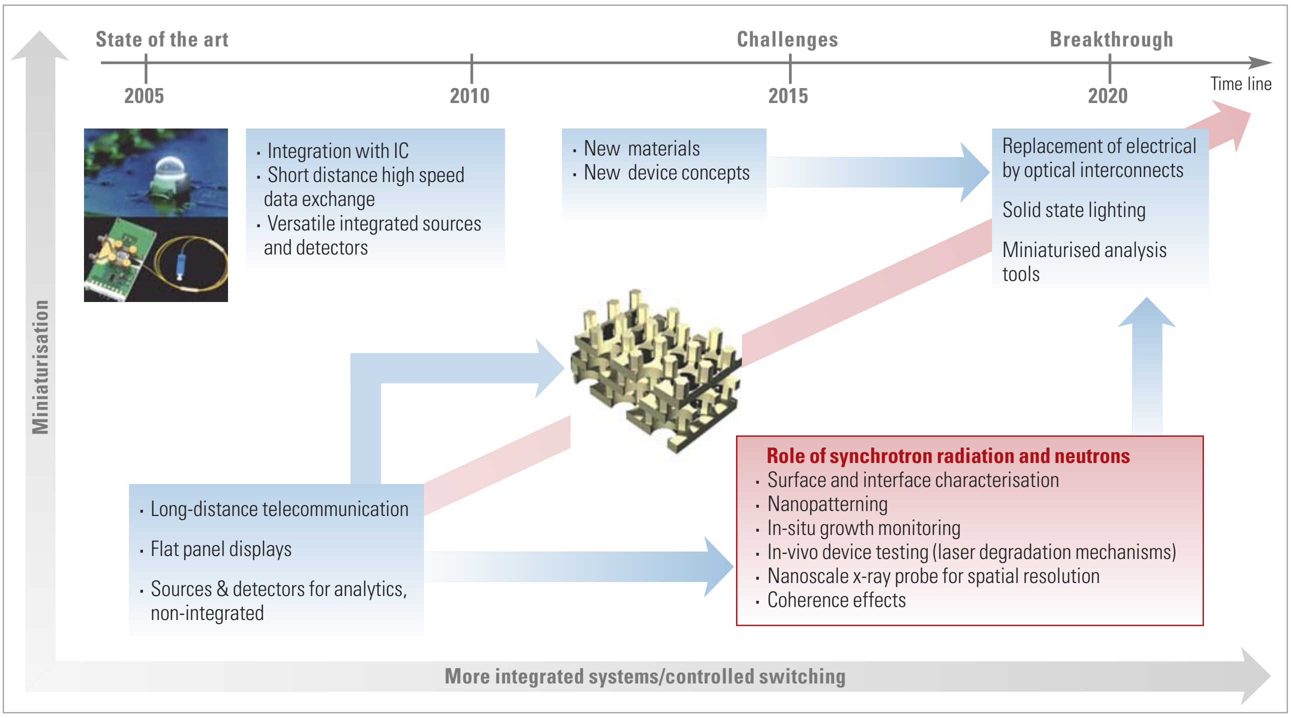

Fig. 3.4.4: Roadmap on the contribution of synchrotron radiation and neutrons towards functional photonic nanomaterials research.

Non-linear optical devices

Non-linear optical devices, which control light with light, are required for all-optical logic devices and for ultimate ultrafast optical communication. In addition to the synthesis of optical materials with large non-linearity, the development of optical cavities based on photonic crystals or plasmonics is required for obtaining large electric fields.

Nanostructures for ultrasensitive chemical analysis

Giant electric field enhancement in photonic crystals or plasmonic crystals is expected to bring novel methodologies for ultrasensitive chemical analysis. Research on biochips or establishment of environment analysis processes, which enable high speed detection of arbitrary molecules in a small volume with very low concentration, is vitally important.

Exploitation of the quantum nature of photons

The quantum nature of photons will be brought into use. Entangled photons are indispensable for quantum computation and quantum cryptography. In particular, realisation of strong light-matter interaction, e.g., based on the combination of quantum dots and photonic crystal cavities, is of prime importance. Single photon sources, which generate non-classical light, would also be utilised as a new class of light sources.

STATE-OF-THE-ART

PHOTONIC NANOMATERIALS

Photonic crystals (PC)
Artificial opal
Colloid crystal
Photonic crystal slab
Photonic crystal fibre
Diamond structure
Simple cubic structure

Metamaterials
Plasmonic nanostructure
Negative index material
Chiral structure
Random and fractal structures

Microcavities
Microsphere
Microdisc
Micropillar
Micropyramid
Photonic crystal cavity

Quantum nanostructures
Quantum well
Quantum dot (QD)
Quantum ring

Measurements
Near field scanning optical microscope (SNOM)
Single dot spectroscopy

Unusual phenomena
Photonic bandgap
Modified Planck's law
Purcell effect
Smith – Purcell radiation
Classical localisation of photon
Small group velocity
Enhancement of:
- non-linear optical processes
- stimulated emission
- optical bistability

Waveguides with sharp bends
Super continuum generation
Super prism
Super lens
Negative refraction
Surface enhanced Raman scattering
Quantum confinement of exciton & biexciton
Rabi oscillation
Strong coupling
Rabi splitting

FUTURE NEEDS AND CHALLENGES

MAIN RESEARCH ACTIVITIES

Fabrication
- Sophisticated lithography:
  - Electron beam
  - Focused ion beam
  - Ultraviolet & x-ray
- Controlled self-organisation:
  - STM assisted positioning of QD
  - Vertically coupled QDs
  - Anodic oxidation
  - Semiconductor nano"molecules"
  - Quantum double rings
  - Remote fabrication in SEM

Characterisation
Further development of:
- Probe microscopes
- Single dot spectroscopy
- Single molecule spectroscopy
- Single photon spectroscopy
- Photon correlation
- Fourier spectroscopy
- Ultrafast spectroscopy

Cavity QED
- Development of high-Q PC cavity
- QD – PC coupled structure
- Quantum gate operation

Applications
Super continuum light source
- PC fibre-based:
  - Gas sensor
  - Laser surgical knife
- PC-based:
  - Optical microcircuit
  - Optical microcomponent
  - Ultra-fast optical switch
- QD laser:
  - QD-based biomarker
  - Multi-frequency optical communication

Novel phenomena
Quantum localisation of photon
Optical detection of single spin
Single molecule Raman scattering
Single photon propagation in PC
Entanglement of remote QDs
Excitonic Aharanov – Bohm effect
Controlled NOT gate

FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRON SOURCES

SYNCHROTRON RADIATION
- Material characterisation: defects, interfaces, especially for monolithic integration
- Organic materials development: stability in time-resolved studies, dependence of stability on structure
- In-situ growth monitoring to understand growth phenomena and improve growth techniques
- In-situ device testing, change of properties and degradation of devices during operation, needs non-destructive technique

NEUTRONS
- Systematic neutron studies of electron-phonon interactions to reveal the dephasing mechanism in quantum nanostructures
- Quantum "optics" of neutrons

Fig. 3.4.5: Opportunities for synchrotron radiation and neutron techniques in the field of photonic nanomaterials.

3.4.3. MATERIALS FOR NANOMAGNETISM AND SPINTRONICS

The discovery of the interlayer exchange coupling in magnetic superlattices in 1986 and the giant magnetoresistance (GMR) effect in 1988 can be considered as the starting points of what is known today as nanomagnetism. The challenge now is to go into 3-D arrays of magnetic nanobits for increased storage capacity. The 'race-track' memory device, advocated by IBM, is the first 3-D concept.

The ever increasing need to store and process data has fuelled applied and fundamental research in probing the temporal and spatial limits of magnetic switching. Exploring the magnetisation in MRAM-bits by applied magnetic field pulses is a very active research field involving real-time studies of synchrotron based time-resolved spectro-microscopy. Novel switching phenomena based on angular momentum transfer from a spin polarised electrical current are beginning to be explored. A completely new field is being developed where information transfer is no longer based on charge transport leading to heat dissipation problems, especially in nanosized structures. Instead, in AC spin currents, spin transfer phenomena across – and spin accumulation at – interfaces, play an increasingly important role in many spintronics applications for nanoscale objects.

Key future needs for advanced analytical techniques are (see Fig. 3.4.6):

- The determination of coupling angles and domain structures in magnetic heterostructures and superlattices;
- The precise measurement of magnetisation profile in dilute magnetic semiconductors;
- The real-time measurement of magnetisation reversal and domain formation in exchange-biased systems;
- The microscopic understanding of proximity effects in spring magnets.

A fundamental understanding of the microscopy of the magnetic state of nanomagnets is needed to discover new phenomena. To this end, it is of critical importance to characterise and elucidate the physical and chemical factors that control the magnetic properties of nano-assemblies.

The need for synchrotron radiation and neutron facilities for future research and development of nanomagnetic materials

Synchrotron radiation and neutrons provide unique analytical access to magnetic systems; they have been vital for the present understanding of magnetism, in particular in complex, small and low-dimensional systems (see Fig. 3.4.7). In nanomagnetism, it is essential that synchrotron radiation and neutrons will offer clever new analytical solutions for the study of: i) smaller scale objects, ii) on a shorter timescale and, iii) with higher precision.

A major impact of synchrotron radiation and neutrons is expected from:

- Time-resolved experiments on magnetic nanostructures down to pico- and/or femtosecond resolution;
- Ultrahigh resolution studies of the electronic structure, giving new insight into coupling phenomena and revealing the electronic origin of the anisotropy of magnetic materials;
- Stroboscopic spectroscopy and nanodiffraction experiments using pump-probe type excitations (temperature, magnetic field);

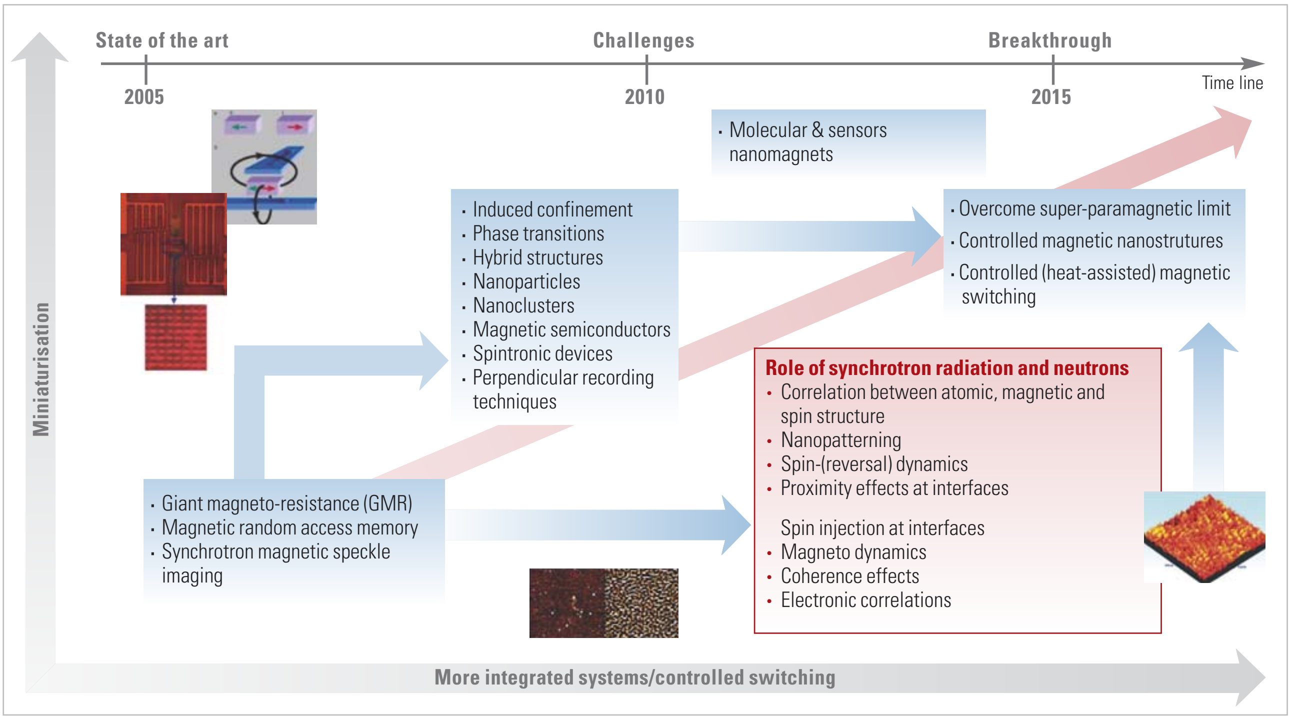

Fig. 3.4.6: Roadmap on the contribution of synchrotron radiation and neutrons towards functional magnetic nanomaterials research.

STATE-OF-THE-ART

Magnetic materials and properties
Magnetic semiconductors
Magnetic vortices
Quantum transport
Confinement structures:
- Clusters (size, interdistance)
- Nanopillars & nanoarrays
- Nanowires
- Nanocontacts
- Molecular nanomagnets

Complex heterostructures
New spintronics systems
Manipulation of spins
Organic spintronics

Synthesis
Self-assembled growth
Nanoscale lithography
Upgraded cluster techniques
Computer simulation

Industrial application
Electronics:
- MRAM
- Magnetic recording
- Device switching

Spin – FET, Spin – LED
Biomedicine:
- Drug delivery
- MRI

FUTURE NEEDS AND CHALLENGES

Nanomagnetism
Magnetic phenomena:
- Phase transitions in confinement (dimensional crossover)
- Anisotropy
- Domain wall propagation
- Magnetic roughness
- Exchange bias
- Magnetisation switching
- Spin transfer and dissipation

Nanomagnetic materials
Hybrid structures:
- FM/Semiconductor
- FM/Insulator/FM
- FM/Superconductor

Nanoparticles & clusters

Magnetic semiconductors:
- Magnetic tunnel junctions
- Spin dependent transport

Advanced characterisation
Enhanced microscopic understanding of:
- Nanostructure and magnetism
- Spindynamic in nanoconfinement
- Effect of impurities
- Magnetic polarisation of embedded atoms
- Local contribution of spin and orbit to magnetic moment

Industrial application
New spintronic devices

FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRON SOURCES

Exploration of new nanomagnetic materials
Characterisation of:
- Superlattices and interfaces
- Nanoscale phenomena
- Hierarchical materials
- Magnetic semiconductor
- Magnetic viruses
- Dynamic effects (down to fsec timescale)

Development of new instrumentation and techniques
Complimentary instrumentation integration
Synchrotron radiation, neutrons and other techniques (MOKE, MFM, SNOM, SEMPA)

- Specular reflectivity/off-specular scattering
- New beam line SR PEEM/XMCD
- Micro- and nanodiffraction (time-resolved)
- Magnetic nanospectroscopy (soft x-rays; also time-resolved)
- Lens-less imaging (time-resolved)
- Pump-probe experiments (at neutron spallation sources and FEL's)

Fig. 3.4.7: Roadmap: Opportunities for synchrotron radiation and neutron techniques in the field of nanomagnetic materials.

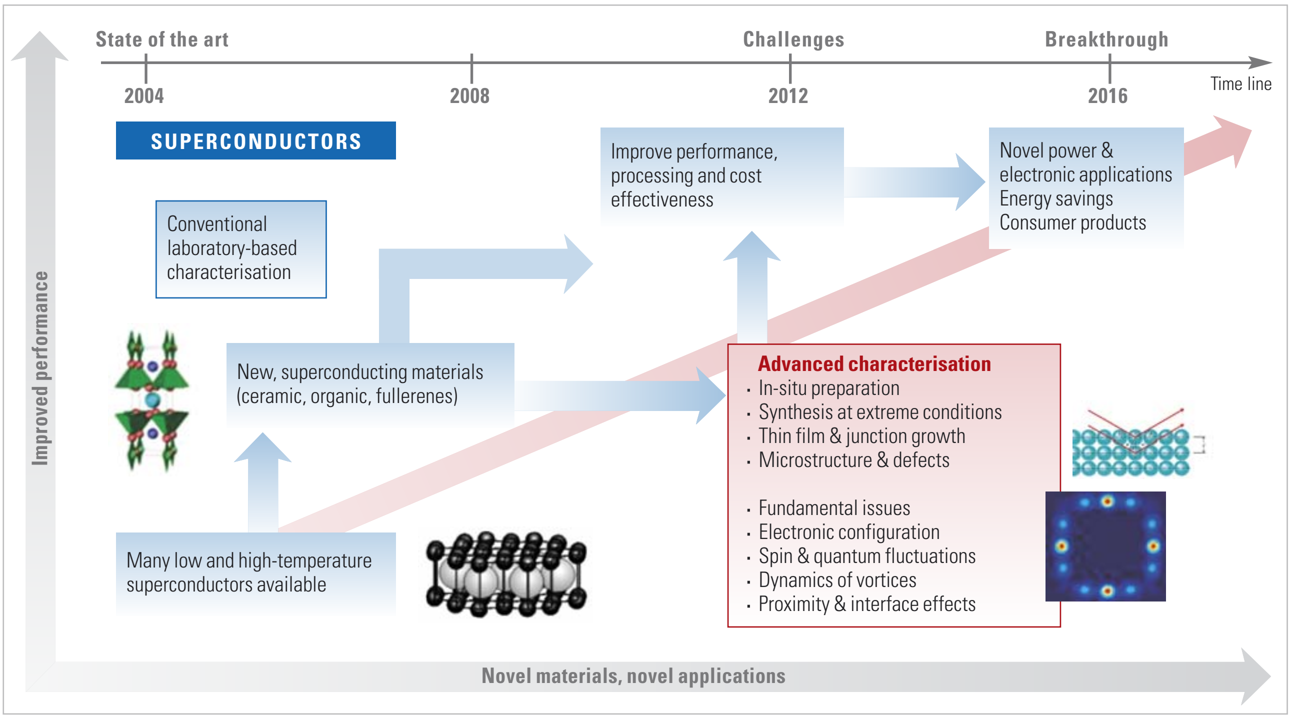

Fig. 3.4.8: Roadmap on the contribution of synchrotron radiation and neutrons towards superconductor nanomaterials research.

- Monitoring of interfacial diffusion and reactions at interfaces of metal and organic multilayers on the nanoscale;
- Systematic studies of spin-structures and spin-fluctuations in artificial superlattices and laterally patterned arrays.

3.4.4. SUPERCONDUCTORS

The discovery of oxide high-temperature superconductors (HTCS) in 1986 has given the field a major new stimulus. However, HTCS present a multitude of materials problems at the atomic or nanometre scale that have to be solved in order to optimise them for practical use. Most of today's superconducting devices are still based on conventional superconductors. Present applications involve solenoids, ranging from small magnets for academic research to huge systems for large laboratory facilities (accelerators). The biggest actual market is for superconducting magnets used in medical diagnosis, in particular Magnetic Resonance Imaging (MRI).

Breakthroughs

Breakthroughs in the field of superconductors are intimately related to progress in materials research. The technical performance of HTCS is often superior but production and material costs are still too high. The preparation of bulk superconductors presents particular material problems that are intimately linked to their functionality. In thin-film

STATE-OF-THE-ART	FUTURE NEEDS AND CHALLENGES	FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRON SOURCES
New superconductors HTC: · Cuprates (YBCO & BSCCO) LTC : · MgB_2 · Intercalated bucky-balls · Heavy fermions · Ruthenates · Boron-doped diamond **Advanced synthesis** Nb-Ti, Nb- Sn, Nb-Al BSCCO-2212/BSCCO-2223 YBCO-coated conductors Single crystals growth High-quality thin films Nanoscale materials **Superconducting devices** Multiple-barrier heterostructures Planar multiple-barriers Nanoscale heterostructures SFS & SFNFS junctions **Applications** Power cables: · Accelerators; MRI, motors, generators, condensers, transformers,etc. Electronics: · Filters · Josephson devices (SQUIDS)	**MAIN RESEARCH ACTIVITIES** **Materials-related issues** Search for new superconductors New synthesis & doping techniques Defects and microstructure Nanomaterials Nanomanufacturing **Fundamental science issues** Electronic structure & quasi particle dynamics: Magnetism and spin fluctuations Quantum fluctuations Strong correlations Vortices Single vortex physics Multi-vortex physics Proximity and interface effects Non-equilibrium effects Spin injection **Nanostructured superconductors** New phenomena & processes Tunnel-junctions Nanowire networks Heterostructures & superlattices Nanoclusters **Advanced synthesis & doping techniques with in-situ control** Thin film growth Synthesis at extreme conditions Bulk samples, single crystals, thin films Atomic-layer engineering Combinatorial materials science High-throughput screening Field-effect & photo-doping **Advanced characterisation of properties** Chemical & structural composition Ultrathin films Hybrid structures Magic nanoclusters Nanowires "Stripe"- order formation Spin fluctuations Electron-phonon interaction	**Fundamental aspects** · Exploration of the HTC coupling mechanism · Systematic neutron studies of electron-phonon interaction · Soft x-ray spectroscopy and x-ray diffraction to explore the coexistence of magnetism and SC (ARPES, XES, RIXS, HREELS, XAFS, ITS) · Exploration of quantum fluctuations with neutron and x-ray spectroscopy · Systematic exploration of thin superconducting films and interface phenomena using grazing incidence diffraction and spectroscopy **Novel materials** · Dedicated x-ray and neutron beam lines for high throughput studies of novel SC materials · Dedicated x-ray and neutron beam lines for combinatorial materials science

Fig. 3.4.9: Opportunities for synchrotron radiation and neutron techniques in the field of superconducting nanomaterials.

HTCS, there are many examples of how non-thermodynamic compounds can be stabilised through epitaxy with substrate or buffer layers. Of particular interest in the search for new materials is the phase spread method, where composition gradients in thin films are intentionally introduced. Structural characterisation of such layers during growth requires in-situ technologies with a high level of sensitivity and reliability. These technologies can be provided by synchrotron radiation and neutron facilities (see Fig. 3.4.8).

Role of synchrotron radiation and neutron facilities
(See Fig. 3.4.9) Developments in spectroscopy and electron microscopy (e.g. new detectors) and different scattering techniques (x-ray and neutrons) at the nanoscale will in parallel ensure our ability to study structure and bonding and, ultimately, obtain an atomic level relation between structure and function. As the limits of performance are pushed, the figures of merit of nanostructured superconductors (junctions, wires, clusters, etc.) need to be optimised. Knowledge about the (sub-)microscopic nature of the structures and how they evolve is crucial. This requires detailed high-resolution characterisation of the microstructure of the devices and a high level of correlation between structure, property and fabrication parameters.

The prime analytical technologies are:

- Angle Resolved Photoemission (ARPES)
  For the future, many developments can be expected in ARPES. With higher resolution, it will become possible to explore: (i) mean free paths for the low energy excitations comparable to those measured in transport, (ii) the spin charge separated components to the point where we can look at the temperature dependence of each separated component.
- Neutron scattering
  Neutron scattering has played a central role in cuprate studies yielding many spectacular successes including the anti-ferromagnetic parent state and its destruction by hole-doping, the observation of ‘stripes,’ and universal spin excitation structure. Neutron scattering studies of the cuprate and other exotic superconductors will play a central role in the future of the field.
- Resonant X-ray Scattering (RXS)
  RXS investigations (elastic and inelastic) will become increasingly important for the study of electronic ordering near buried interfaces in materials that have been nanopatterned. Improved scattered energy analysis will also allow for detailed study of `fluctuating' order. The use of high magnetic fields will allow the study of field induced charge ordering in vortices.

3.4.5. CARBON NANOMATERIALS

The discoveries of fullerenes in 1985 and of carbon nanotubes (CNT) in 1991 opened a completely different perspective from that of carbon materials based on flat graphite-like hexagonal layers. Carbon nanotubes have particularly attracted the attention of many scientists in the wide fields of science and technology as an important compo-

STATE-OF-THE-ART	FUTURE PROSPECTS	FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRON SOURCES
Carbon nanomaterials Model system: · Basic science · Nanotechnology Building blocks: · Integrated devices · Nanoelectronics · Nanoelectromechanics · Nanooptics · Nanofluids **Fullerenes** Endohedral systems Polymerised phases (1-2-3 D) Structural perfection Adsorption & storage possibilities Carbon nanotubes & peapods: · Ideal model as 1D-solid · High structural perfection · Unique structure & chemical stability Interesting physical properties: · Metallic · Semiconducting · Magnetic · Superconducting	**Carbon nanotubes** **Research activities** Controlled growth & production: · Nanotubes with defined length, diameter and helicity · Optimise chemical doping · Upgrade self-assembly · Separate metallic/semiconductor structures Fundamental properties: · Confinement-related effects · Electrical, magnetic, optical, mechanical and thermal · Correlation between atomic structure and electronic properties · Inter-tube coupling **Potential applications** Composite materials Adsorption & storage devices Electrical & mechanical systems Battery electrodes Field emitters Chemical sensors Catalysis Field – effect – transistors Printing – memories – logics	**New synthesis & doping techniques** In-situ analysis to achieve: · Controlled growth and hybrid structures · Production of high quality & quantity · Synthesis in extreme environments · Upgrade purification & separation · Optimisation of self-assembly · Optimisation of chemical doping of peapods · Fabrication of high-strength fibres · Nanofluid structures **Novel properties** Advanced characterisation of: · Chemical & structural composition · Nanotube-polymer composites · Transfer processes · Interactions metal-nanotube, molecule-nanotube · Electron excitation dynamics · Architecture of integrated nanotubes devices · Nanotube-based opto-electronic devices **Particular challenges** Single molecule diffraction and spectroscopy: · Tailoring of nanobeams · Controlling radiation damage (x-rays) · Time-resolved diffraction and spectroscopy experiments · Inelastic neutron spectroscopy for thermal excitations in CNT arrays

Fig. 3.4.10: Opportunities for synchrotron radiation and neutron characterisation methods for research on carbon nanomaterials.

nent in the realisation of nanotechnology. The synthesis of carbon nanotubes can be accomplished by a wide variety of methods that involve the catalytic decomposition of a carbon-sample-containing gas or solid. Some of the most common techniques are chemical vapour deposition, arc-discharge, and laser vaporisation synthesis. Nanostructured films with controlled architectures are desirable for many applications in optics, electronics, biology, medicine, and energy/chemical conversions. Low-temperature, aqueous chemical routes have been widely investigated for the synthesis of continuous films, and arrays of oriented nanorods and nanotubes.

The amazing mechanical and electronic properties of the nanotubes stem from their quasi one-dimensional structures and the graphite-like arrangement of the carbon atoms in the shells. Thus, CNTs have high Young's modulus and tensile strength, which makes them preferable for composite materials with improved mechanical properties. The nanotubes can be metallic or semiconducting, depending on their structural parameters. However, with our present knowledge of the nanotube growth process, control of these parametres has not yet been accomplished. This control will eventually open the way for application of nanotubes as central elements in electronic devices, including field-effect transistors (FET), single-electron transistors and rectifying diodes (see Fig. 3.4.10 and 3.4.11). In addition, graphene sheets – one atom thick two-dimensional layers of carbon – offer interesting physics due to the fact that the charge carriers are massless Dirac fermions. Apart from its remarkable electronic properties, graphene-based composite materials offer widespread applications e.g. as polystyrene-graphene composite for conductive plastic materials, as graphene powder for improving the efficiency of batteries, as graphene sheets for solid state gas sensors.

3.4.6. DIELECTRIC MATERIALS

Advanced dielectric materials are a prerequisite for the improvement of future Si-based micro- and nanoelectronic integrated circuits (ICs) so as to achieve improved performance, and higher functionality. Today, the semiconductor industry is paving the way for the transition from micro- to nanoelectronics. This, in turn, will allow for the further improvement of the performance of Si-based IC's. In accordance with the International Technology Roadmap for Semiconductors (ITRS), the development of new dielectric materials will be among IC manufacturers' primary goals in making the production of Si-based nanoelectronic devices feasible. In this race for capitalising on research breakthroughs, synchrotron radiation and modern neutron sources have a large potential to keep the "time-to-market" periods of the technology short and European IC manufacturers competitive.

Future research needs and analytical challenges (see Fig. 3.4.12)
The research and technology areas of high priority to achieve an in-time transfer of basic research results on dielectric nanomaterials into Si-based micro- and nanoelectronic technologies are:

- To optimise dielectric film preparation and processing techniques
  - Film deposition techniques with atomic control for research and industrial needs;

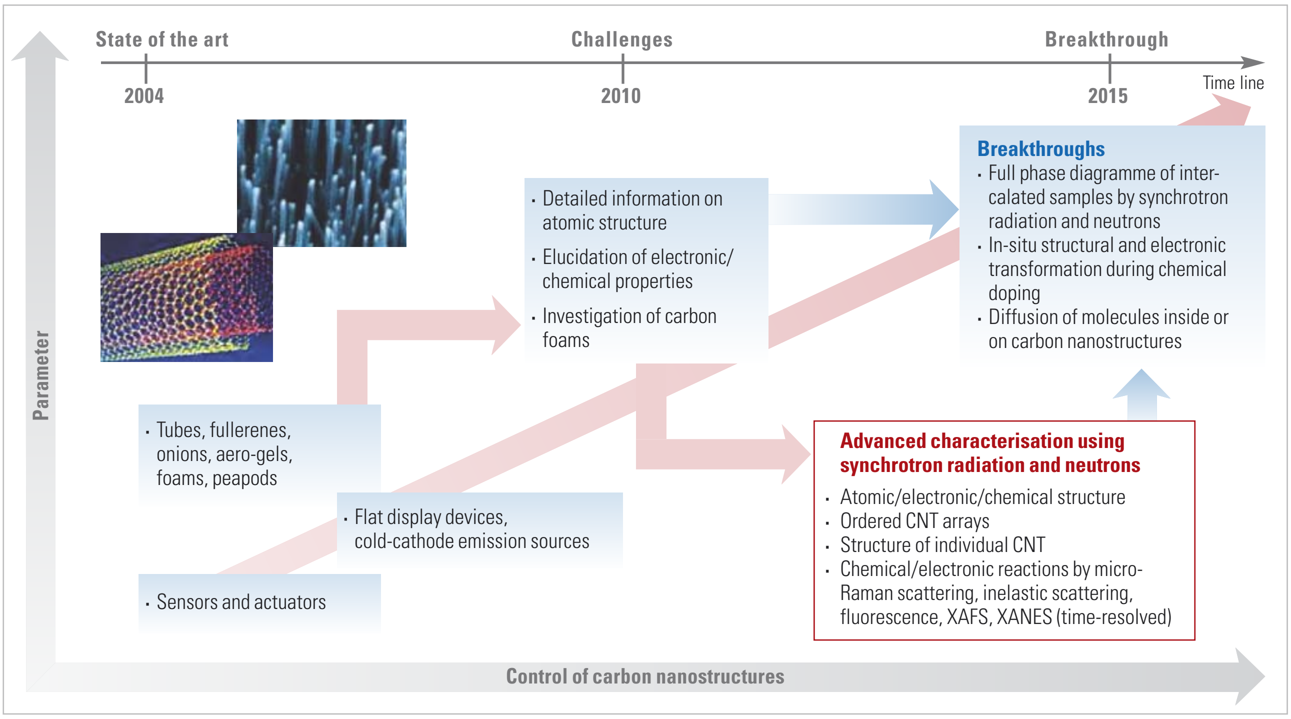

Fig. 3.4.11: Roadmap for future research on functional carbon nanomaterials.

- Adaptability of "state-of-the-art" machinery to integrate dielectric nanomaterials in Si-based nanoelectronic devices.
- To develop characterisation methods for dielectric nanomaterials
  - Techniques with high spatial, time, and energy resolution,
  - High sensitivity for defect engineering,
  - On-line diagnostic capability etc.
- To study materials science of dielectric nanomaterials
  - to tailor dielectrics on the nanoscale;
  - to evaluate emerging materials concepts for device applications;
  - to study the fundamental/theoretical understanding of nano-dielectrics.

Future role of synchrotron radiation and neutron facilities

Synchrotron radiation and neutron facilities are of key relevance in the successful development of advanced dielectrics for Si-based micro- and nanoelectronic ICs. In order for Europe to keep a world-wide competitive position in the nanoelectronics technology, the European Commission must promote the innovation of this important sector of nanomaterials development and encourage a new partnership between university/industry and the synchrotron radiation and neutron facilities. The synchrotron radiation and neutron facilities in turn must provide brilliant beams in the energy ranges of interest, and detectors with fast electronics and high dynamic range for nanoscience studies.

The specific needs for the development of advanced dielectrics are:

- High spatial resolution diffraction and spectroscopy beam lines for micro- and nanobeam studies;
- Dedicated beam lines for non-destructive depth profiling of thin films with highest sensitivity to defects;
- Experimental set-ups for high resolution spectroscopy and diffraction studies.
- To reduce "time-to-market" periods for new nanodielectrics in Si-based micro- and nanoelectronics, the infrastructure of large scientific test facilities should be adapted and upgraded to the requirements of the IC-industries, requiring:
  - Improved beam time access and use by technology-oriented allocation procedures, user-friendly control and data handling software;
  - Synchrotron radiation and neutron beam lines with new level of automatisation and standardisation.

3.4.7. CONCLUSIONS AND RECOMMENDATIONS

The properties of synchrotron radiation and neutrons present enormous potential for research and the promotion of innovation in the large field of functional nanomaterials:

- Studying fundamental mechanisms at the atomic level
- Unraveling the complexity in novel materials
- Tuning of functionality

SCIENCE

- Tailoring devices
- Processing
- Fabrication

INNOVATION

This implies that synchrotron radiation and neutron centres will naturally become a focus for the nanomaterials research and technology in Europe. The competitive scientific and industrial interests will push the existing infrastructure capabilities such that it will provide:

Cross-fertilisation

- More intense collaboration between various research communities and industries;
- Technology and knowledge-transfer through multi-disciplinary research & development.

Infrastructure

- Real time, in-situ experiments – down to sub-picoseconds;
- Nanoscale focus of experiments – spatial resolution better than 10 nanometres;
- Atom-selective spectroscopy – ability to resolve microscopic environments;
- Surface and interface sensitive diffraction and spectroscopy experiments – essential for the study of the all important interfaces of composites;
- New imaging, tomography and microscopy techniques;
- Soft (destruction-free) probes for organic and biological nanomaterials.

Public awareness

- Make facilities attractive to young scientists, non-specialists, commercial/industrial clients;
- Provide more/better training programmes;
- University "road-shows".

Scientific breakthroughs

- Clarify how electronic, optic, and magnetic properties depend on atomic structure (3-D atomic structure of superconductors, carbon nanotubes, magnetic materials, usually cannot be determined by other techniques);
- Identify the bottlenecks in material and device design (by defect characterisation, in-situ and in-vivo characterisation, measurement of otherwise inaccessible material properties in the material volume);
- Develop "local diffraction probes" by nanobeams, to combine and correlate spatially resolved diffraction and imaging results with other locally resolving methods like microscopy, micro-photoluminescence (this will, in the near future, only be possible at synchrotron radiation sources);
- Investigation of buried interfaces in composite materials, which are most of the functional materials discussed. This can only be achieved with synchrotron radiation and neutron scattering. Nanotechnology aims also to imitate natural materials, which are to large extent composite materials, where the interface properties dominate or entirely determine the material properties!

The impact of synchrotron radiation and neutron on the development of new functional nanomaterials is given in the following diagramme (see Fig. 3.4.13).

FUTURE APPLICATIONS

LOGIC DEVICES
Silicon-on-insulator (SOI)
Low-k interlayer dielectrics
High-k gate dielectrics
Ferroelectric gate dielectrics

MEMORY DEVICES
High-k materials
Dynamic Random Access Memories (DRAM) and Flash cells
Ferroelectric materials
Ferroelectric Random Access Memories (FRAM)
Various dielectrics
Tunnel oxides for Magnetic Random Access Memories (MRAM)
Phase Change Random Access Memories (PCRAM)
Holographic data storage
Switching oxides, etc.
Wireless communication
Dielectrics for Metal-Insulator-Metal (MIM) capacitors
Surface Acoustic Wave (SAW)-filters
Data transmission
Microwave communication systems
Nanoelectronics interfacing
Diagnostic devices
Lab-on-chip solutions
Sensors
Electronic noses
Pyroelectric IR-detectors
Tactile sensors
Integrated nanosensors

RESEARCH AND DEVELOPMENT

PREPARATION
Deposition
Atomic scale control
(mass flow, oxygen pressure, etc)
Research
Flexibility for materials screening
Industry
High mass flow for production
Processing
Top-down and bottom-up approaches

CHARACTERISATION
Dielectric techniques
Leakage, dielectric constant and loss, defects and interface states
Materials science techniques
High sensitivity
Non-invasive character
High spatial resolution
High energy resolution
On-line diagnostics
High time resolution

MATERIALS
Experimental
Materials manipulation on the nanoscale
(global and local approaches etc.)
Materials for new device concepts and physics
(oxide electronics, spintronics, orbitronics etc.)
Theory
Growth kinetics
Thermodynamics
Electronic properties etc.

CHALLENGES FOR SYNCHROTRON RADIATION AND NEUTRONS

SENSITIVITY
Machine
Adequate brilliance in the different energy ranges
Detectors
Fast electronics of high dynamic range

RESOLUTION
Spatial resolution
Beamline optics for micro-and nanobeam studies
Experimental techniques for non-destructive depth profiling
Energy resolution
Experimental set-ups for high-resolution spectroscopy and diffraction studies

VARIOUS
Beam line access
Technology-oriented evaluation procedure
Quick access upon demand for successful proposals
User friendliness
ISO-certified beam lines control and data handling software

Fig. 3.4.12: Dielectric nanomaterials for future Si-based micro-and nanoelectronics. Challenges for synchrotron radiation and neutron facilities.

FUNCTIONAL NANOMATERIALS

TOPIC
- Quantum data
- Complex integrated (hybrid) devices
- Nanocrystals

PROBLEM
- How to sort out information on very small areas from average sample properties

SOLUTION
- Focusing of x-ray beams to 10 nm range enable combined direct space & reciprocal space solution

TOPIC
- Semiconductor heterostructures
- Organic compounds
- Composite materials

PROBLEM
- How do properties depend on interface structure

SOLUTION
- Scattering experiments using synchrotron radiation and neutron scattering
- Access buried interfaces destruction-free, in-situ if required

TOPIC
- Magnetic materials
- Superconductors
- Dielectrics

PROBLEM
- How do material properties depend on atomic structure

SOLUTION
- Diffraction studies with synchrotron radiation and neutrons sensitive to particular properties (magnetic moment, crystal structure, surface reconstruction)

TOPIC
- Photonic materials
- Integration of optics & electronics
- Degradation of materials during use

PROBLEM
- What are the bottlenecks limiting material and device properties and design

SOLUTION
- In-situ and in-vivo studies during material fabrication and device operation

Fig. 3.4.13: Schematic overview for the needs of synchrotron radiation and neutrons.

Overall guidelines for synchrotron radiation and neutron facilities

Several specific measures and recommendations for the future use of synchrotron radiation and neutrons can be formulated, corresponding to different timing periods for both policy makers and facilities.

In the short term:

- Upgrade existing sample environment: low temperatures, high magnetic fields and pressures, availability of in-situ growth chambers;
- Install secondary lab-based characterisation techniques for simultaneous measurements;
- Improve detector technology: 2D-detectors, He 'hemispherical' detectors, faster read-out, better dynamic range etc.
- Develop hybrid scattering experimental techniques;
- Facilitate combined use of neutron and synchrotron beam lines (not absolutely necessary – the samples can also be transferred but this should be facilitated);
- Stimulate the interaction between modelling methods to the experimental measurements, with a longer term view of using the predictive capabilities to direct experiments in nanomaterials sciences;
- Increase attractiveness for non-specialist users (for instance by providing user-friendly sample environment and automatic data analysis procedures) and to create a fast access lane for exceptional exploratory test experiments;
- Users would welcome faster turn-around times between submission of project proposals and actual experiments at the synchrotron radiation and neutron facilities. The long delay between submission of proposals, uncertainty of approval and eventual allocation of beam time makes the incorporation of synchrotron radiation and neutron experiments into any research project unattractive. Nevertheless, there are provisions for industrial projects at any synchrotron source to get speedy access and turnaround. Basic research projects just need to be of sufficiently high scientific quality.

As a long-term project, there should be a considerable investment in the infrastructure: new dedicated beam lines and detector development, creation of 'Centres of Excellence' in specific nanoresearch fields, user-support facilities.

Most of the leading industrial research is already carried out outside of Europe and it may be expected that the European neutron drought will undoubtedly lead to a similar situation for academic research.

Europe has to present all the effort needed to allow it to maintain its position as a global leader in the development of novel LINAC-based x-ray and neutron sources.

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3.5.1. FROM POLYMERS TO BIOLOGICAL SYSTEMS

Self-assembly of soft matter, such as amphiphilic molecules, block copolymers, surfactants, etc., into supramolecular structures offers an unprecedented variety of morphologies that can be used to create nanoscopic structures and functionalities. The self-assembling process rests on the fine balance of competing interactions between the different molecular parts or different molecules that exhibit similarities to complex biological systems. The control of this molecular self-organisation by means of chemical and physical stimuli is the key to the successful creation and control of structure on the nanometre and micrometre scale. The use of self-assembly ranges from the development of new formulations for pharmaceuticals and pigments to morphology control, adhesion of biomaterials, the development of molecular electronics and biomimetic crystallisation.

Fig. 3.5.1 gives an overview of nanostructured biomaterials and Fig. 3.5.2 exemplifies the importance of self-assembly in the context of nanomaterials.

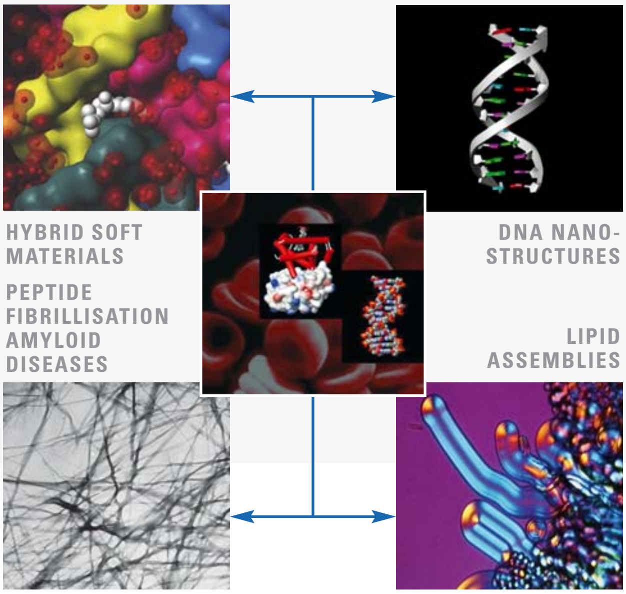
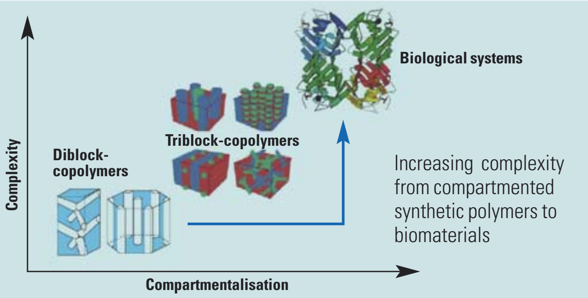


Fig. 3.5.1: Overview of nanostructured biomaterials.

TEMPLATING NANODEVICES

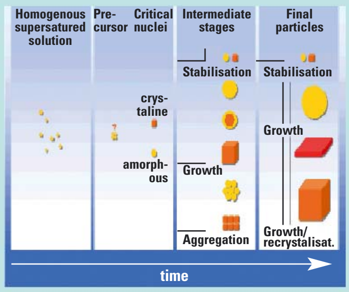
- Formulation of pharmaceutical drug carriers
- Mesoporous structures for separation technologies
- Morphology control of biomaterial adhesion
- Catalyst support materials
- Magnetic storage devices
- Molecular electronics
- Photonic materials



Increasing complexity from compartmented synthetic polymers to biomaterials

PARTICLE FORMATION

- Formation process of nanoparticle pigments
- Protein or polymer-guided biomineralisation



Structure formation during particle formation processes from super-saturated systems. By knowledge of the molecular mechanisms, it will be possible to control the process by design.

SMART AND FUNCTIONAL MATERIALS

- Responsive hydrogels
- Electro- and magneto-rheological fluids
- Nanocomposites
- Hybrids of synthetic and biological matter

Fig. 3.5.2: Self-assembly to create nanostructured materials: research goals.

Templating nanostructures through self-assembly (Fig. 3.5.2)
Self-assembling block copolymers offer an unprecedented variety of morphologies and control routes by appropriate nanoengineering. The self-assembly process rests on the fine balance of competing interactions between the different polymeric parts, and exhibits similarities to complex biological systems. In the bulk, diblock copolymers can self-assemble into four different structures. Together with a silicon precursor, a variety of nanoscale structures may be achieved. Via the control of polymer chemistry and processing conditions, the nano-objects are predetermined in size, shape and composition. Meso-porous materials for separation technologies and highly efficient catalysts are obtained. The polymeric templates may be extended to biology, including systems to direct cell or issue response for biocompatibility in biosensor applications. Other applications in medical science include implants, prostheses, drug delivery and diagnostics. The future potential of the self-assembly approach for the

creation of new nanomaterials lies in the versatility of polymer chemistry in connection with, for example sol-gel chemistry, which may be exploited for synthesis. The addition of further soft materials adds to the parameter space of complexity.

The platform of structures challenges the use of such polymer systems as new structure-directing agents for novel nanostructured materials. Depending on the hard component to be introduced, templating of magnetic devices, smart materials, photonic crystals, and membrane structures for gas separation in fuel cell applications is conceivable.

Research potential for synchrotron radiation and neutrons
- Neutron and x-ray small angle scattering interrogates mesoscopic structures and component behaviour.
- X-rays are sensitive to the hard components.
- Neutrons address the soft matrices.
- Contrast variation using neutron scattering by component deuteration highlights partial structures.
- In-situ x-ray and neutron investigations allow quantitative monitoring of the effect of structure formation under external fields.
- Magnetic neutron scattering addresses the magnetic structures of soft and hard composites.

Nanoparticles
Another issue is the creation of well-controlled nanoparticles, particles in the range of about 10nm to a few 100nm. They influence our lives in the form of protein complexes; as viruses; as colloid particles in drinking water, surface water, and sea water; and as aerosols. They find use as dispersion colours and as adhesives. In industry, they play an important role in the formulation of pigments and in the production of catalysts. Numerous attempts are being made to deliver nanoparticulate forms of pharmaceutically active compounds specific to the desired site of action in the body. Finally, the use of nanoparticles as quantum dots with special properties for electronic components is also a target area.

Many active organic materials are poorly soluble or even insoluble in water. Aqueous forms for application thus require special formulation techniques in order to be able to utilise or optimise physiological (pharmaceuticals, cosmetics, plant protection, nutrition) or technical (varnishes, printing links, toners) function. The most interesting properties of nanodispersed, active organic materials include the impressive increase in solubility, the improvement in biological resorption, and the modification of optical, electro-optical, and other physical properties that are achievable only with particle sizes in the middle or lower nanometre range. In this context, attention is drawn to the recent increase in research activities that have as their objective the continuous, automatic preparation of nanodispersed systems by precipitation from molecular solution. This undertaking is complicated by the complexity of many precipitation processes, which extends far beyond the currently used picture of nucleation and growth.

Research potential for synchrotron radiation and neutrons
- Neutrons and x-rays provide information regarding heterogeneous particle structures through contrast variation and selective labelling.
- Neutron and x-rays provide in-situ structural information on particle growth.
- Neutrons and x-rays allow the in-situ exploration of kinetic pathways.
- Neutrons allow clarification of the role of different components in complex formulations by selective labelling.
- Neutrons address magnetic structures including domain formation in magnetic nanoparticles.

Biomineralisation
Inorganic materials are an important component of biological systems, e.g. calcium carbonate and calcium phosphate crystals in skeletal structures. These crystals are formed in the presence of biological macromolecules, which constitute an important part of the emerging structures. The methods by which living systems have generated and handled these materials are often very intricate and are only just starting to be understood. What is clear, however, is that the synthesis, transport, aggregation and final deposition of these nanocrystals involves a complicated sequence of interactions with bio-macromolecules. If understood and mastered, biomimetic biomineralisation will offer a new approach to novel nanostructured composites and functional materials that are presently beyond reach.

Research potential for synchrotron radiation and neutrons
- The complementary use of x-rays and neutron allows soft and hard components to be distinguished in biomineralisation processes.
- X-rays and neutrons facilitate an in-situ observation of biomineralisation kinetics including the evolving structures.
- X-rays and neutrons offer the opportunity to investigate morphology textures and the response to external forces.
- X-rays and neutrons together allow pinpointing the role of biopolymers.

Nanocomposites
Hybrids of crystalline inorganic particulates and polymers are being developed to combine the advantage of both classes of materials and to widen their range of applications. Enhanced mechanical, dielectric fire resistance, heat deflection, and permeation barrier properties have been reported and can be expected, though the basic mechanisms and microscopic understanding is underdeveloped. The properties of such nanocomposites relate to those of the individual components, composition, structure (spatial distribution), particle-particle interaction and particle-matrix interaction.

Research potential for synchrotron radiation and neutrons
- The complementary use of neutrons and x-rays distinguishes the soft and hard domains.
- By specific labelling, the response of the soft matrix to external forces may be directly measured.
- Neutrons can address the dynamic properties of the composites.

- Neutrons provide direct insight into the change of polymer conformation in the presence of hard components.
- Neutrons address the segmental and global dynamics of polymeric components.
- Contrast variation and selective labelling allows separation of the structure and dynamics of different soft components in complex composites.

Protein-based nanomaterials

Protein-based soft nanomaterials are of great interest for medical applications. There are many cases where it is necessary to organise the structural arrangement of proteins, e.g. in cell scaffolds. In therapeutic applications, the peptide should be targeted to a particular host. Both of these objectives can be achieved using soft matter self-assembly, specifically by using polymers as templates or supports.

Understanding aspects of protein self-assembly is still a huge and vital challenge,e.g. to understand protein folding is one of the main outstanding questions in biology. Soft matter science has much to offer in understanding this (see Fig. 3.5.2).

Research potential for synchrotron radiation and neutrons

- Synchrotron x-ray and neutron scattering are powerful techniques to probe the nanostructure of such biomaterials.
- Synchrotron SAXS will enable high resolution experiments or fast time-resolved studies, e.g. of protein folding. Fourth generation facilities may be important in such studies.
- Neutron scattering will facilitate the precise elucidation of structural details via contrast variation and specific labelling experiments.

DNA-based nanomaterials

DNA can be used in biosensors and even as scaffolds to programme designer self-assembled nanostructures. Of course, it is also a very important high density information storage material. Its incorporation into integrated circuits is currently under investigation. It is indeed a key structural element in bio-nanotechnology.

Research potential for synchrotron radiation and neutrons

- Small-angle scattering of x-rays and neutrons will be essential to characterise self-assembled structures in solution and during processing.
- The recognition behaviour of arrays of DNA-functionalised nanoparticles could be probed by in-situ time-resolved scattering experiments.
- The self-assembly of designer DNA fragments into intricate nanostructures could be investigated by specific labelling.
- Grazing incidence diffraction could provide information on DNA nanostructures on silicon substrates.

Overall potential for synchrotron radiation and neutron research

Nanoscale systems and devices involve complex materials usually containing different nanophases. Their structure can be unravelled by neutron scattering and, in particular, by small angle neutron scattering (SANS). Neutrons enable us to probe structure on distance scales spanning the entire nanoscale regime: atoms to macromolecules. In addition, the large cross-sectional difference for hydrogen and deuterium, enables H/D labelling studies of complex "soft", biological and "soft-hard" nanosystems. This isotopic labelling can also be used to highlight particular interfaces of nanosystems involving "soft" components (see Fig. 3.5.3). Moreover, many nanodevices contain magnetic phases. Neutron scattering has proven to be the unique tool for the investigation of the magnetic structure of matter, both static and dynamic (fluctuations).

Small angle x-ray scattering (SAXS) as performed at a synchrotron has the advantage of very high flux, permitting measurements on extremely short timescales (this is state-of-the-art) as well as high resolution studies. The ability to perform fast, time-resolved measurements is very relevant to in-situ studies of nanostructure formation and processing. The latter is needed to fully probe the structure of ordered DNA or protein assemblies.

Understanding the mechanisms of nanostructuring in biological and biomimetic materials, and in particular the processes of self-assembly, is of the utmost importance in the development of new products and technologies. Future developments will move towards the study of increasingly complex, often multi-component systems, where time dependent phenomena in real-time experiments, non-equilibrium situations and transient phenomena will be the focal point. Enhanced flux neutron and x-ray scattering will be needed in order to follow these processes in real-time. This is of particular relevance in the case of "soft" nanosystems, e.g. organic nanoparticles and self-assembling polymer templates. The ability of neutrons to penetrate macroscopic flow devices will allow exploration – in real-time – of actual industrial processing mechanisms. Enhanced synchrotron radiation techniques are expected to lead to breakthroughs in understanding the mechanisms of protein folding, peptide fibrillisation, DNA nanostructure formation etc. Here again, there is huge potential for in-situ measurements on samples under flow, in electromagnetic fields or other processing conditions.

The nanoscale experiments described above involve small samples, complex molecules, time-dependent aspects of synthesis or self-organisation and weak interactions. While modern synchrotron sources provide fluxes that are already at the limit of or beyond what organic or biomaterials are able to bear before being destroyed, neutron experiments are very often flux limited. Most experiments we can envisage are at the limit of present-day capabilities or they are simply impossible. Thus, the future development of the field strongly demands high flux neutron sources such as SNS or the planned European Spallation Source. In the synchrotron field, methods of development such as the use of coherent beams will significantly enhance the capability of European synchrotron facilities.

Conclusion

The self-assembling properties of soft condensed matter constitute a field of large breadth and richness of phenomena with many potential technical applications in nanoscience. X-rays and neutrons play a key role for the exploration of this field (see Fig. 3.5.3). The advantages of neutrons are simultaneous accessibility to the proper length- and time-scales, together with a possibility for changing the scattering contrast.

Future developments will move towards the study of increasingly complex, often multi-component systems, where time dependent phenomena in real-time experiments, non-equilibrium situations and transient phenomena will become the focus.

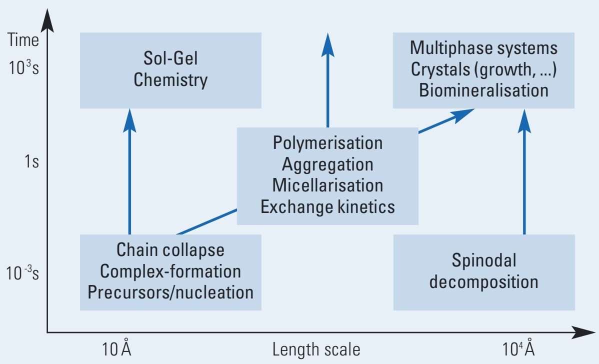
X-ray and neutron scattering, in combination with computer simulations, will have a very large impact on all these future endeavours. All the future trends require a strong increase in the available neutron intensity, which will be provided by the planned upgrades of the ILL instrumentation and to an even larger extent by the upcoming MW-neutron spallation sources presently being constructed in the USA and Japan and planned for Europe.

Synchrotron x-ray techniques will enable major breakthroughs in understanding the self-assembly of soft matter relevant to various medical, sensor and IT technologies.

TEMPLATING OF NANODEVICES

A rational design of such materials will need a detailed characterisation of all components. Small angle neutron scattering and neutron reflectometry using selective labelling, contrast variation and possible polarisation analysis will offer unparalleled means of investigating self-assembled structures. In concert with other techniques such as synchrotron radiation, NMR and imaging methods, the information necessary for a thorough understanding will be obtained.

The structural complexity together with multidimensional parameter space will require extensive sets of experimental data necessitating high flux instrumentation. Furthermore, investigations into the kinetics of structure formation will need fast diffraction experiments.

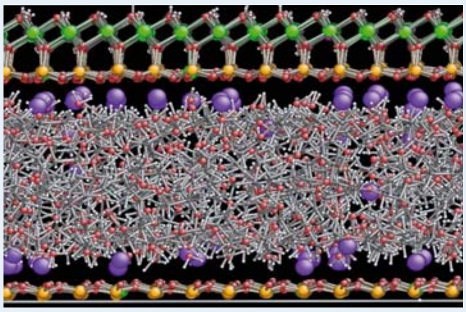


NANOSCALE PROCESSING

Specific labelling and the large penetration depth of neutrons are both essential in revealing information on detailed structure and mutual interactions. This knowledge is necessary in order to understand and control the subtle interplay between components in such systems. Moreover, it will be necessary to follow the formation of self-organised systems with the necessary time resolution. This is a very interesting problem that is also directly related to recent progress in material sciences (novel non-metallic materials, ceramics processing, food science and technology etc.). However, this requires time-resolved SANS and SAXS experiments on the second and millisecond timescale. Again, the potentially much higher fluxes of next generation neutron sources would elevate the possible impact of research in this area.

NANOCOMPOSITES

X-ray and neutron scattering are particularly sensitive to the macromolecular component of the composite structure. They provide a unique tool to follow the evolution of the microstructure of these materials; both the degree of dispersion heterogeneties, and orientation may be followed in-situ during extrusion and further optimised.



Non-linear mechanical properties are poorly understood, but of great industrial interest. They could be directly accessed on a molecular scale relating molecular motion and displacement to mechanical properties.

NANOPARTICLE FORMATION

SANS and SAXS are unique techniques to characterise nanoparticulate formulation, since most systems consist of at least three components (water, active ingredients, stabilising polymers or surfactants). Insight into structural features is gained by contrast variation – either by D_2O/H_2O exchange or by selectively deuterating one of the components. SAXS at synchrotron radiation can be carried out with sub-sec time resolution. Future high flux neutron sources will pose the opportunity for time-resolved SANS studies. Only then will it be possible to really understand the formation processes in nanoparticulate systems and to develop new ideas and products based on this knowledge.

BIOMINERALISATION

Similar to the case of nanocomposites, neutron scattering, in particular, addresses macromolecular components, specifically utilising contrast variation of the aqueous environment. This applies also to biomimetic crystals grown in-vitro in the presence of macromolecules or other large organic molecules.

Fig. 3.5.3: Impact of synchrotron radiation and neutron investigations.

3.5.2. BIO-NANOMATERIALS

Materials used by nature are composed of nanosized building blocks, such as proteins, filaments, membranes or mineral particles. They fulfill vital functions in living organisms from energy conversion to chemical synthesis and mechanical stabilisation. Typically, these nanostructures are assembled into larger assemblies, such as tissue, following hierarchical principles. This gives control over the structure and dynamics of biomaterials over many length scales, and is a major concept for designing artificial multi-functional and adaptive materials. Understanding the principles of hierarchical assembly in living organisms and applying them to engineered materials and structures is – and will be in the future – the grand challenge of nanomaterials research (see Fig. 3.5.4).

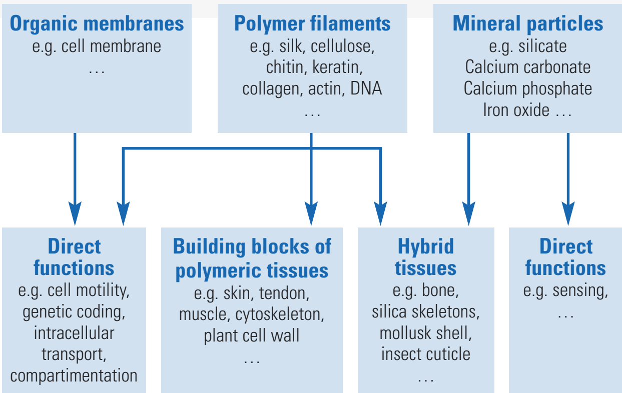


Fig. 3.5.4: Types and functions of biological materials.

Three major research directions can be identified in the field of hierarchical biomaterials (see Fig. 3.5.6).

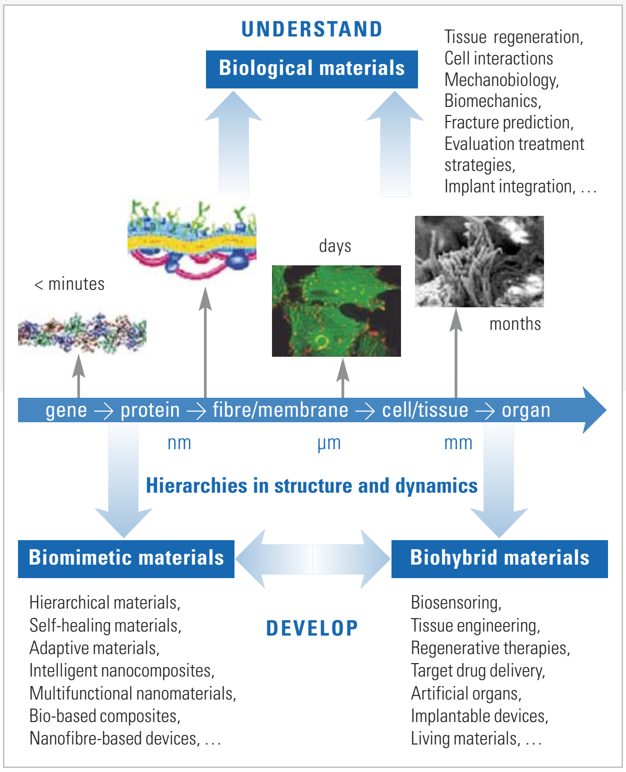


Fig. 3.5.6: Overview of research directions in bio-nanomaterials.

The use of artificial nanomaterials (semiconductors and metallic particles) is envisaged in future biomedical applications (light-sensitive markers in biological tissues, externally addressable devices using magnetic or electric fields in living organisms). Research on (artificial) organic or inorganic nanoparticles will provide new strategies for drug delivery, biosensing, diagnosis and treatment of disease. In most cases, these nanomaterials will be used in hybrid devices and revolutionary novel properties and combined functionalities will be achieved. This will make the traditional classification of materials in metals, ceramics, semiconductors and polymers obsolete (see Fig. 3.5.5).

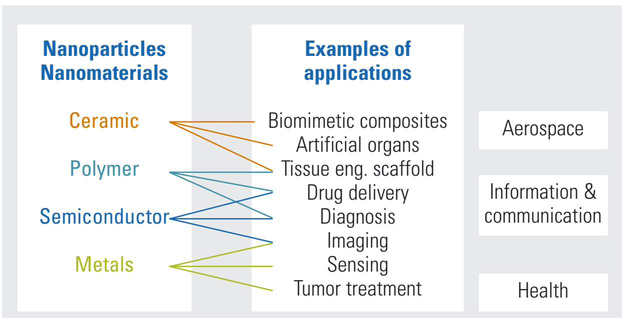


Fig. 3.5.5: Current and future applications of nanoparticles and materials based on nanosized building blocks.

Future research in bio-nanomaterials

- Improve the understanding of natural nanostructures;
- Systematic study of the relation between function, structure and dynamics in biological materials (plant bodies, cells, extra-cellular matrix, intracellular materials);
- Understand synthesis, adaptation and healing strategies used by nature to build, maintain and repair these usually very complex materials.
  - Direct applications in biomedicine,
  - Impact in cellular and structural biology,
  - Input into biomimetic materials research.
- Use this knowledge to create new artificial materials:
  The development of bio-mimetic materials is based on the understanding of how natural materials work. This type of research will lead to the development of novel materials such as polymers, ceramics, metals and composites with new properties, e.g. multifunctionality, self-healing capability, adaptability, etc. Such materials will find applications in many different fields, from biomedicine (e.g. implants, organ replacement) to transport technology (e.g. aerospace) and information technology (e.g. nanomotors, nanofluidics, molecular electronics, etc.). The ultimate grand challenge is to assemble artificial functional units which reproduce the functionality of cells or even organs (artificial life).

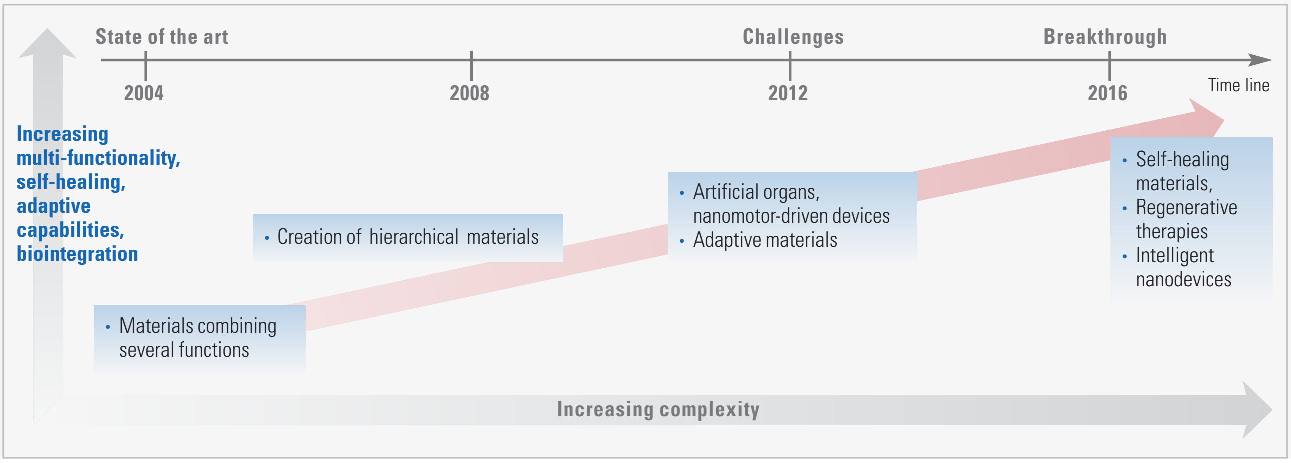


Fig. 3.5.7: Roadmap for research in bio-nanomaterials

- Create hybrids between biological and artificial materials: With the widespread effort to develop new strategies for regenerative medicine, there will be the need for a range of new materials that can be integrated as hybrid structures into living systems (scaffolds for tissue engineering, in-vivo implantable permanent biosensors, drug carriers, materials for bioreactors and artificial organs).

Future challenges

For all three research directions, nanomaterials play a crucial role, as most of the biological materials are based on nanometre-size building blocks. However, it will be essential to investigate not only nanoscale characteristics, but also a wide range of dimensions since most bio-related materials and devices cover multiple length scales to develop their functionality. Understanding and creating hierarchical structures from the nano- to the macro-range is one of the current challenges.

Synthesis	Characterisation	Properties & functions	Prediction of properties
Hierarchical materials	Multi-scale characterisation	Understand biological nanomaterials	Multi-hierarchical modelling
Self-assembly at various scales	Time-resolution	Knowledge-base for multi-functionality	Modelling many timescales
Specific particle shapes	In-situ experiments	Concepts for adaptivity	Quantitative modelling of adaptive behaviour
Biointegration	In-vivo measurements	Concepts for self-healing	Modelling multi-functionality
Co-synthesis of hybrids	Marker-free measurements	...	...
...	Quantitative analysis		
	...		

Fig. 3.5.8: Research needs in bio-nanomaterials.

Further challenges include the development of adaptive and self-healing materials, of strategies and materials for regenerative therapies, and of new strategies for imaging, sensing as well as diagnosis and treatment of diseases (see Fig. 3.5.7).

These challenges imply a major research activity in materials research, from synthesis and characterisation to theoretical modelling and the development of new concepts for structure and function. Systematic research is mandatory to be able to synthesise, characterise and model materials which are hierarchical in nature. In turn, all these experimental and theoretical concepts must cover a large range of dimensions and timescales. Strong efforts are necessary to render bio-nanomaterials suitable for new applications, in particular in health, aerospace and communication technologies (see Fig. 3.5.8).

Importance of synchrotron radiation and neutron research for bio-nanomaterials (Fig. 3.5.9)

The characterisation of the hierarchical processes and structures of biomaterials requires a dedicated use of synchrotron radiation and neutron techniques. It is mandatory that biological structure-property relations are determined by in-situ methods, where a specimen is being studied in a time-resolved way during a chemical reaction, a phase transformation or during the response to an external stimulus, such as changes in temperature, magnetic field and mechanical load.

- Multi-scale synthesis and characterisation (of structure, properties and their inter-relation) must go hand in hand for efficient research and development in the field of bio-nanomaterials;
- Research on bio-nanomaterials conducted at any European or national research institution needs equipment with a variety of characterisation techniques, such as electron microscopy, NMR and animal test facilities;
- Multi-scale structural characterisation (with spatial and temporal resolution) and marker-free (spectroscopic) characterisation of all synthetic steps requires dedicated beamlines at synchrotron radiation and neutron facilities.

- Microscopic and tomographic structure analysis of cell nuclei, cells, tissue and materials;
- Holographic imaging of materials, nuclei, cells and tissues;
- Scanning diffraction of hierarchical (biological) materials;
- Confocal diffraction of tissues and (biological materials;
- Tracking of nanoparticles inside the nucleus and cytoplasm;
- Time-resolved methods for structure analysis;
- Spectroscopic tools for label-free detection of biomolecules in cells and materials;
- Fundamentals of quantitative spectroscopy in biology, e.g. quantification of radiation effects in synchrotron radiation experiments;
- Quantification of radiation damage in cells and biological materials
- Preparation and manipulation of nanosized specimens with subnanometre resolution;
- Characterise structural and biochemical markers for genetic diseases;
- Comparative studies on cells or subcellular compartments of different mammalian species (mice, rats, etc.) to identify mechanisms of disease development;
- Comparative microscopy and spectroscopy in transgenic animals and plants.

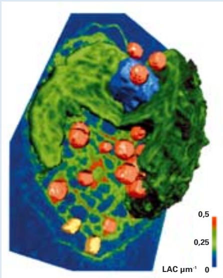


Fig. 3.5.9: Synchrotron radiation and neutrons research in bio-nanomaterials (right: example of a x-ray tomogram of cell organelles in algae taken with a full-field x-ray microscope).

Current barriers for the use of synchrotron radiation and neutrons in life sciences and bio-nanomaterials are:

- The communication barriers between the life sciences, physical sciences and engineering need to be overcome;
- In-house research at synchrotron and neutron facilities is typically not focused enough on modern trends in the life sciences;
- Experiments with biological materials (especially live cells and tissue) require special support facilities and complex specimen preparation environments;
- Presently, insufficient knowledge about radiation damage limits experiments on biological specimens.

Research needs at synchrotron radiation and neutron facilities

- Establish interdisciplinary research centres in the life sciences associated with nearby synchrotron or neutron sources and to large user groups. These centres should provide the necessary life-science competence at synchrotron radiation and neutron centres, provide the biological infrastructure for the experiments and offer their competence to (inexperienced) outside users and to industry. (A model could be the EMBL-DESY collaboration in Hamburg in the field of protein crystallography.)
- Such centres, established at different synchrotron radiation and neutron facilities, should coordinate their research portfolio at the European level.
- Demonstrate and publicise competitiveness and/or cost-effectiveness of the analytical work with synchrotron radiation and neutron facilities in the field of life sciences and biomaterials as compared to traditional laboratory methods.

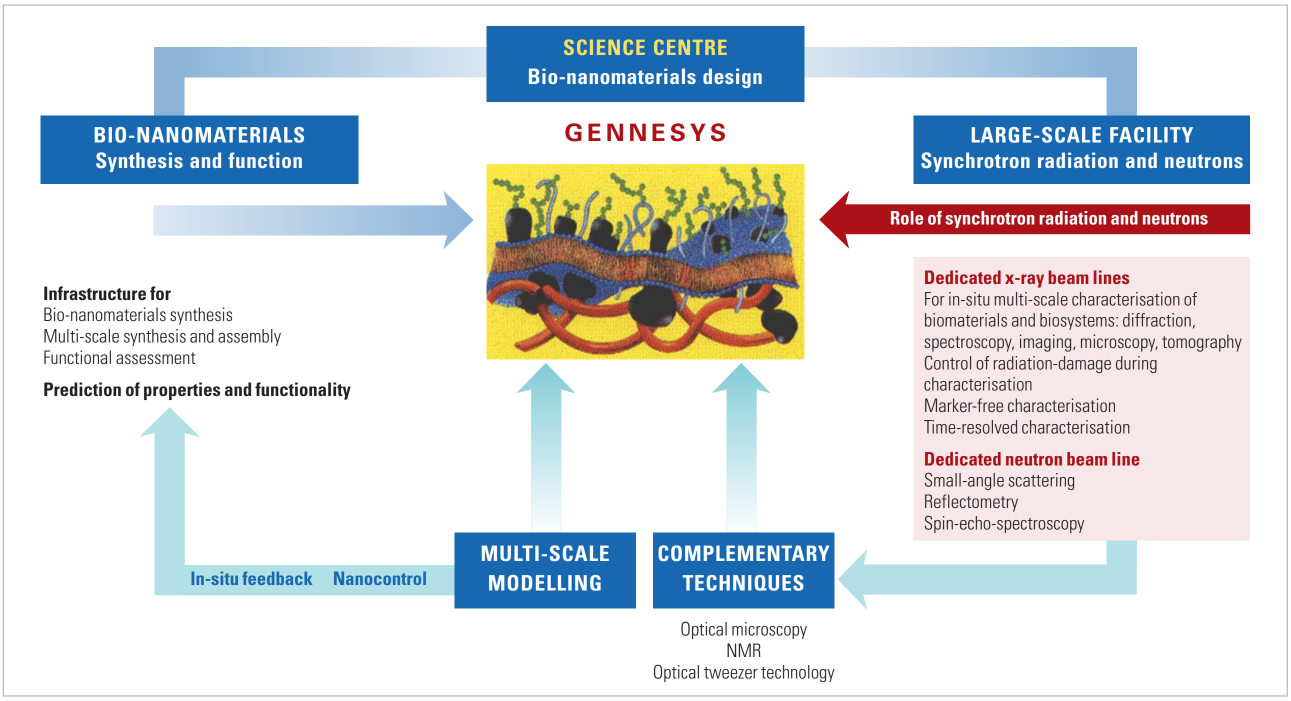


Fig. 3.5.10: Science centre: Bio-nanomaterials design.

- Grants for PhD and/or postdoc positions at synchrotron radiation and neutron facilities should be targeted towards life sciences.
- Sufficient (generous) financial and personnel resources are needed to develop dedicated instruments and specimen environments for the life sciences. The needs of cell and tissue biology should be considered explicitly in the design of new beamlines at the upcoming new facilities.
- Special programmes should be funded to improve knowledge on radiation damage, standardised specimen preparation and handling, standardised data processing and analysis

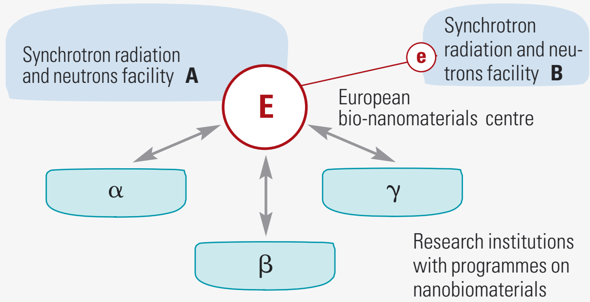
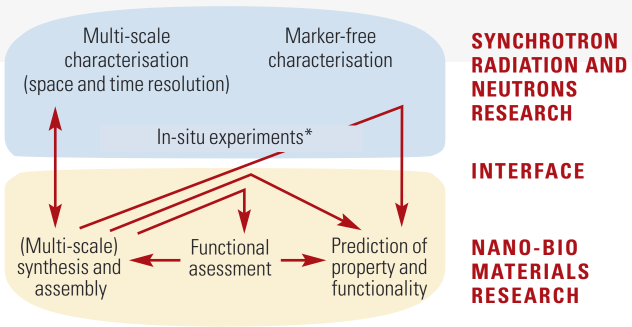


Fig. 3.5.12: Possible mode of operation of a European centre for research on bio-nanomaterials design.



*Structural characterisation e.g. during synthesis or processing or deformation, etc. to elucidate mechanisms of action

Fig. 3.5.11: Multiple and continuous interactions are necessary between research in bio-nanomaterials (yellow) and synchrotron radiation and neutron facilities (blue). These interactions are greatly facilitated by formal collaborations between the research units.

Need for a European centre for bio-nanoresearch
(Fig. 3.5.10, Fig. 3.5.11, Fig. 3.5.12)
The level of interaction between synthesis and characterisation efforts in bio-nanomaterials research requires a different organisation of research at synchrotron radiation and neutron facilities than is common today. Future synchrotron radiation and neutron research on bio-nanomaterials need specialised specimen preparation facilities and sample environments, as well as an enhanced training effort for the users. This can be best implemented by the creation of a bio-nanoscience centre, located at one of the European synchrotron radiation and neutron facilities.

- The centre (E) should be physically located at one of the European synchrotron radiation and neutron facilities, but could have a second site (e) at a further synchrotron radiation and neutron facility.
- The centre must be equipped with state-of-the-art laboratories for bio-nanomaterials research.
- The centre should be run by a minimum of permanent staff responsible for operation and training, as well as conducting their own in-house research.
- Most of the scientists would be short-time visitors (typically one to six months) delegated by research institutions (α – γ) to conduct specialised research using synchrotron radiation and neutrons.

3.5.3. BIOMIMETIC NANOMATERIALS

- Biology (from which biomimetics takes its lead) is predicated on the self-organised generation of function and structure starting at the sub-molecular level. Biological materials grow, though they can be fabricated or assembled (e.g. spinning silk, moulding mussel byssus threads).
- Organisms assemble heterogeneous materials and molecules into functional structures and mechanisms using 'self-assembly' at room temperature and pressure and in an aqueous environment.
- Natural materials are composites based on polymers (proteins and polysaccharides) and some minerals (Ca, Si salts). Metals are but little used as structural materials but can be significant (e.g. addition of 10% molecular Zn or Mn to provide hardened surfaces to insect and spider mandibles; molecular Fe hardening mollusk and fish teeth).
- In their specific mechanical properties, biological materials can match most technical materials (see Fig. 3.5.13), despite the fact that they are based on ceramics (area labeled "1"), polysaccha-

Fig. 3.5.13: Comparison of specific properties of some biological and engineering materials. They cover nearly the same ranges except for high performance ceramics and alloys.

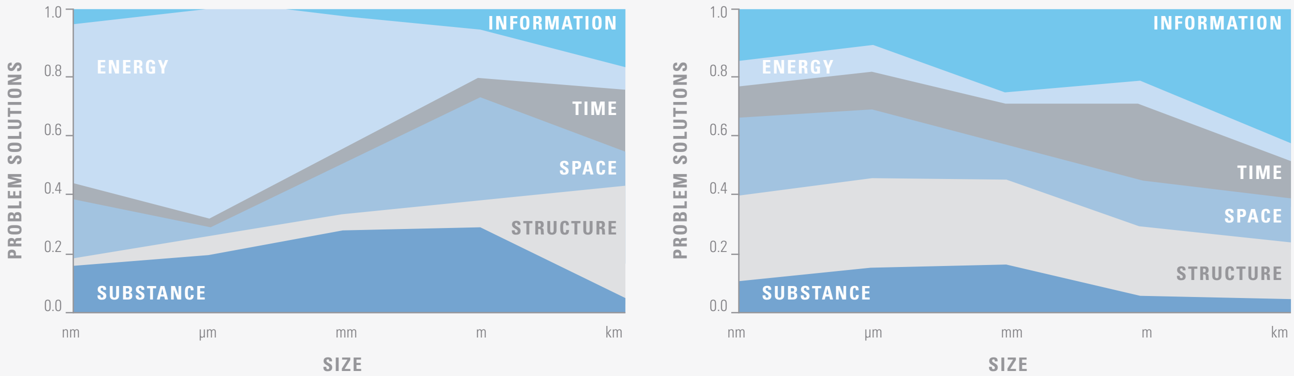


Fig. 3.5.14: How problems in processing are solved in technology (left) and in biology (right). While 70% of the technical solutions involve manipulation of energy (amount, source, type), the use and manipulation of information, from DNA to pheromones, is most important in biology.

rides ("2"), proteins ("3") and highly hydrated materials ("4"). At a given stiffness, biological materials commonly perform better than technical ones in terms of resistance to fracture (toughness) (see Fig. 3.5.16).

- In materials processing, nature replaces the massive use of energy (for example, high temperatures or harsh chemical reactions) with the use of information (equated with structure at all levels, molecule to ecosystem). Indeed, most of the exceptional functionality of biological materials is due to their complex structure, driven by their chemical composition and morphology derived from DNA (Fig. 3.5.14).
- While engineering commonly processes materials by fabrication (e.g. from the melt), biology uses the rich molecular information (composition, arrangement of components, molecular size and shape, hydrophobicity, charge) to direct net forming in growth and assembly processes (Fig. 3.5.15)
- Nature retains hierarchical material structure at all levels since most of the chemical interactions occur over a limited distance. This requires the retention of information (Fig. 3.5.14)
- Natural materials adapt their structure during growth depending on the environment. This is made possible by 'assisted' self-assembly where external forces influence the assembly process (Fig. 3.5.14)
- Adaptation occurs not only in growth but during the whole lifetime of the organism. Cells act as sensors (e.g. for mechanical strains) and add or remove material as needed to adapt to changing environmental conditions (Fig. 3.5.15).
- As a corollary to growth, biological materials and structures are typically self-healing (Fig. 3.5.15).
- By analogy with non-woody plants which experience chronic prestrain of tens of bar, it seems possible that the release of internal prestrain by damage could be regarded as a signal for self-repair.

Hierarchy – function from structure

- The hierarchical structure of biological materials arises from the generation of systems (e.g. wood) resulting from the accretion of subsystems (e.g. cellulose, lignin) during self-assembly and growth. In turn, the systems combine to form supersystems (e.g. tree, forest). As a consequence, adaptation or optimisation of the material is possible at each level of hierarchy. Size differences between hierarchy levels tend to be about a factor of 10.
- The major advantage of hierarchical structuring is that the material can be made multifunctional or that a specific material property, such as fracture toughness, can be improved by optimisation at different size levels. For instance, stiffness is a property controlled at nm levels, whereas toughness (resistance to fracture) is controlled at µm to cm levels. Thus, the two properties can be controlled independently such that biological ceramics can be as stiff as technical ceramics but much more durable (Fig. 3.5.16).

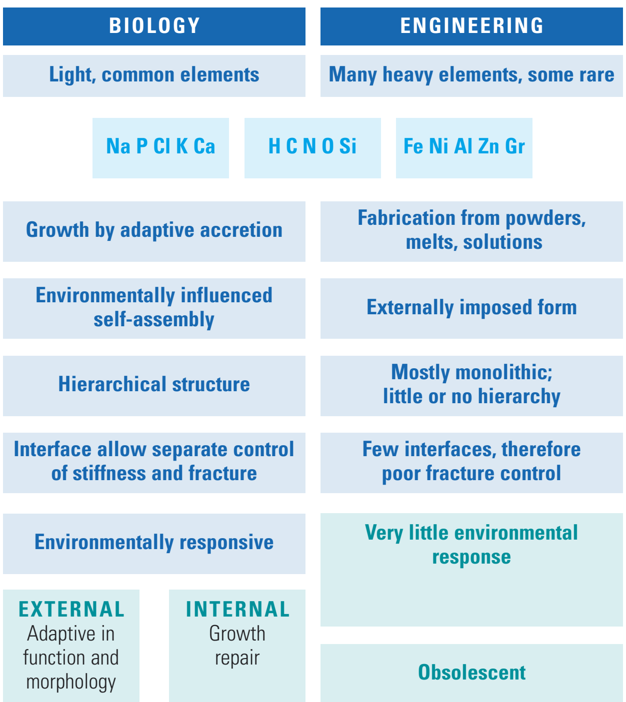


Fig. 3.5.15: Comparison between biological and engineering materials.

- A direct consequence of hierarchy is increased adaptability. Functions can be modified or enriched by structuring at each level of hierarchy. Adaptability increases, therefore, as a function of the number of levels of hierarchy.
- The fabrication of artificial hierarchical structures by top-down fabrication is not generally possible. Bottom-up synthesis remains a challenge if self-assembly is the only technique used. Materials with three structural levels have been obtained by chemical synthesis and self-assembly, up to a size-range of hundreds of nm. However, assembly is possible at greater sizes using appropriate engineering techniques (Fig. 3.5.18), retaining the hierarchical arrangements. Further work in this direction is strongly needed and likely to yield a range of new materials with wide-ranging properties.

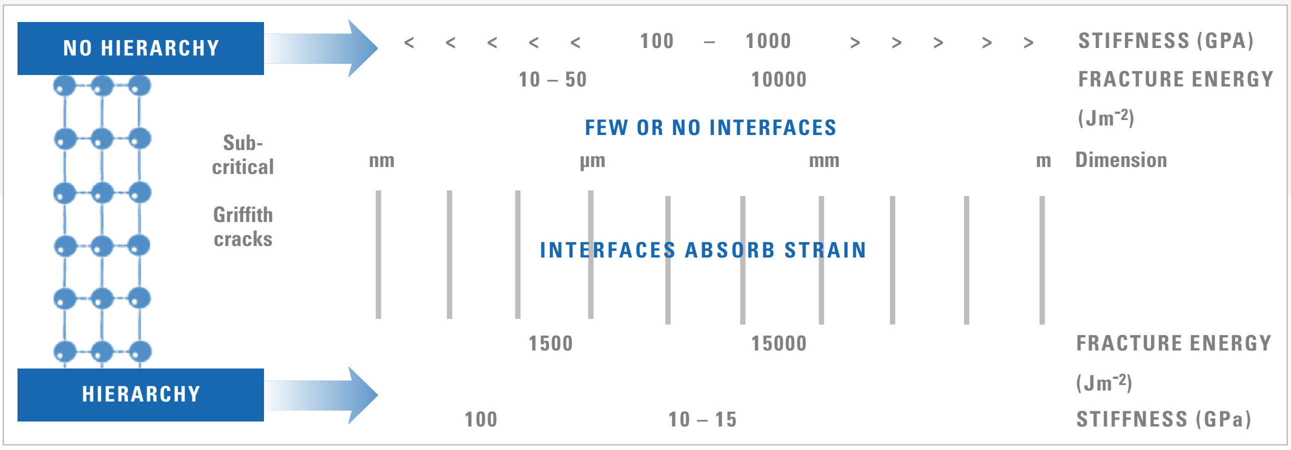


Fig. 3.5.16: The effect of interfaces between level of hierarchy on stiffness (which may fall ten-fold) and fracture energy (which can increase one hundred-fold).

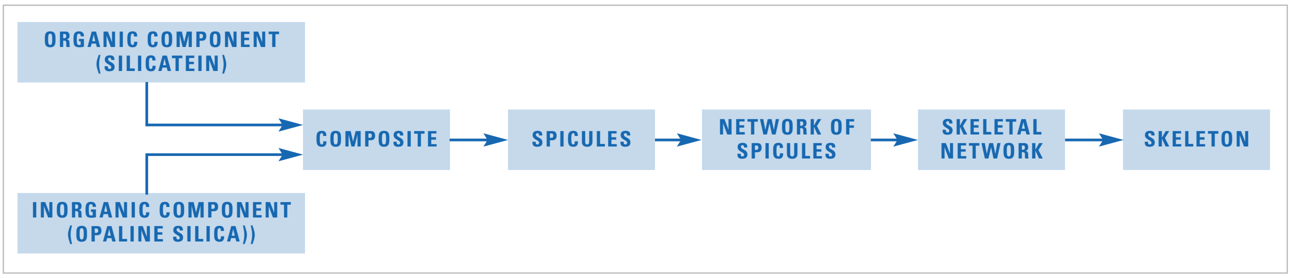


Fig. 3.5.17: Several levels of hierarchy in the structure of the skeleton of the sponge Euplectella.

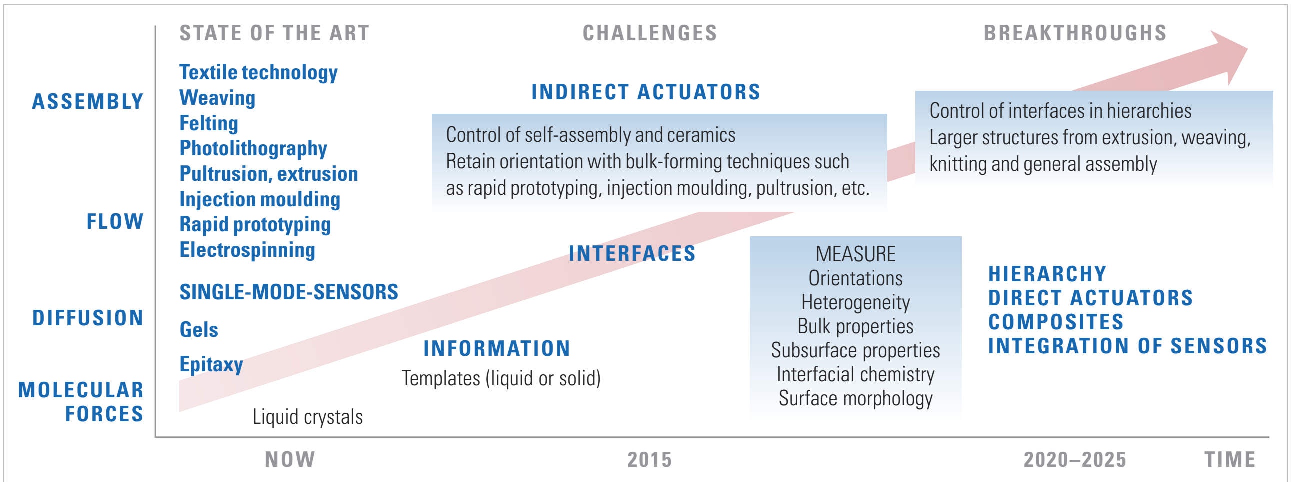


Fig. 3.5.18: Biomimetic nanotechnology roadmap.

- Once hierarchical structuring is controlled in technological processes, it can be used to create new functional materials based on cheap and/or widely accessible base substances. Such materials could be more widely accessible and based on renewable resources. Indeed, it is conceivable to generate materials with various thermal, optical, or mechanical properties, derived from the same base substances. Natural materials, designed from the nm level upwards, provide the prototypes.

Polymers and ceramics

- While structural materials in engineering rely widely on metals and alloys, nature bases all its materials essentially on two polymer families (proteins and polysaccharides) and a range of common ceramics. Important structural proteins are collagen (found, e.g., in tendon and bone), keratin (hair, nails and horn) and silk. Cellulose (predominant in plants) and chitin (in arthropod cuticles) are the most abundant polysaccharides.
- Natural polymer structures produce a far wider range of properties and materials than technical polymers, mainly because of the wide range of morphologies and internal crosslinks made possible by their hierarchical assembly (see above).
- In natural systems, polymers and ceramics are combined in widely differing proportions. Skin or tendon, for example, or the plant cell wall are nearly completely organic, while sea urchins spines and sponge spicules are more than 99% inorganic (made of calcium carbonates and opaline silica, respectively). Bone and dentine are examples of natural ceramics containing more nearly equal amounts of organic and inorganic matter.
- Typically, bio-ceramic structures are much tougher (10 times or more) than technical ceramics. The reason is the intricate structure which is optimised over many levels of hierarchy (Fig. 3.5.17). The skeleton of the Venus Basket sponge Euplectella is made essentially of silica (opal) spicules and gains exceptional mechanical performance by structuring over several levels of hierarchy.
- Like all biological materials, bioceramics are formed under ambient conditions of chemical synthesis.
- Many bioceramic materials contain only very small amounts of polymer usually at the nanoscale and are thus molecular composites. Hence their exceptional toughness.

Biomimetics in action

- Biomimetics involves the transfer of functions from a biological to a technical context. Therefore, it is necessary to be clear about what is being transferred and how to do it.
- There are several levels at which the transfer can be made (Fig. 3.5.19).
- This transfer can be made in a number of ways, from casual inspection to analysis using the Russian system of inventive problem solving – TRIZ.
- Important factors are to be aware of optimisations, context (the best transfer of ideas is made with a context-free environment) and the constraints in both the biological and engineering environments.

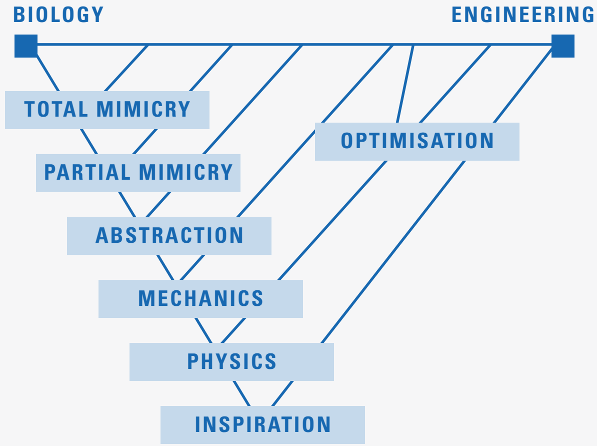


Fig. 3.5.19: Some levels at which ideas, functions or concepts can be moved from biology to engineering.

- Boundary conditions are especially important.
- Natural materials are made from a limited number of basic components displaying a large variety of microstructures. In this way, nature is able to create composite or porous materials with outstanding properties, based on comparatively simple components. One result of this extremely efficient bottom-up "materials design" is the ability to create hierarchical structures adapted to functional requirements at each level of hierarchy. By contrast, current engineering materials have only a limited number of microstructural scales but the variety of potential constitutive materials is enormous. Despite this variety, there are still large blank areas on the materials property charts and materials engineering is constantly facing the challenge of developing materials meeting apparently conflicting requirements.
- By combining the degrees of freedom of hierarchical structuring (inspired by nature) with the variety of materials offered by engineering, there is a huge potential to obtain new or unusual combinations of material functions/properties by structuring a given material, rather than by changing its chemical composition. This is a challenging and potentially highly rewarding research topic.
- Assisted self-assembly, 'state of the art' on the roadmap (Fig. 3.5.18), overcomes a major criticism of self-assembly in general – that it takes too much time. With assistance providing an external energy source, this is no longer an issue.
- Research needs include the characterisation of natural hierarchical materials that may serve as models for the development of biomimetic nanomaterials using assisted self-assembly.
- Research is needed to find and develop principles for designing, simulating and manufacturing biomimetic nanomaterials with property-relevant structural features.
- As nanotechnology can call upon more techniques for synthesizing materials than can biology (which is essentially restricted to ambient conditions of temperature and pressure), the development of manufacturing technologies for biomimetic nanomaterials will be a major research topic.

- Biomimetic nanomaterials may find applications in all technological fields, from electronics (conductors, insulators, superconductors [by self-assembly]), photonics (reflectin platelets stacked giving white reflectance, light guides, non-reflective surfaces, diffraction structures), packaging (materials, sensors), medical (diagnostic, sensing, super-absorbent wound dressing, prostheses, cellular scaffolds for tissue growth), information (actuators, sensors) to security (molecular bar-codes, diffraction structures), as a few examples. Identifying such applications and finding matching solutions based on biological materials is another major activity, which will require, for example, the construction of an ontological data base.

Role of synchrotron radiation and neutrons

- Nature creates materials with outstanding properties and functions by structural hybridisation and hierarchy more than by modification at the chemical level. Thus, structure at all size levels is crucial for these materials. As a consequence, neutrons and synchrotron radiation, which are outstanding tools for structural characterisation, will play a major role in the development of understanding biomimetic nanomaterials.
- Determination of structure-property relations in biological materials and synthetic analogues requires techniques for covering a large range of dimensions, from molecular to millimetric. Both neutron and synchrotron radiation will play a major role. Scanning microfocus techniques will be of particular interest.
- Time-resolved studies of the synthesis of materials, but also material changes due to an external stimulus (light, mechanical stimulus, etc.). Many timescales need to be covered, from electron excitation to slow actuator movements. This implies the use of various (x-ray and neutron) spectroscopies, time-resolved scattering, etc.
- Biomimetic nanomaterials are extremely heterogeneous and need a multi-method approach for characterisation. Synchrotron and neutron methods need to be complemented by other (e.g. spectroscopic or scanning probe) methods. Development of in-situ combinations will be useful (e.g. synchrotron combined with Raman spectroscopy acoustic microscopy, etc.)
- Three-dimensional characterisation with high-resolution: x-ray and neutron microscopy/tomography, confocal diffraction, etc. Further development of cryo-techniques to reduce radiation damage.
- Development of special specimen environments to allow for in-situ characterisation during synthesis, transformation, switching etc. under nearly native conditions.

General conclusions and recommendations

A variety of challenges have to be addressed in the field of biomimetic nanomaterials:

- It is necessary to study a significant selection of natural materials in order to elucidate how they are structured by nature to achieve unusual property combinations;
- Theoretical and experimental tools of materials science need to be developed to address the issue of hierarchical structuring, of multi-functionality and adaptivity of this type of materials;
- New approaches for design, synthesis and processing of biomimetic materials and demonstrators have to be developed (see Fig. 3.5.20).

1) Structure-function relation in selected biological materials

The structures we observe in natural systems are most probably good solutions that emerged after a long adaptation process during evolution. Unfortunately, we do not know exactly which problem has been solved. The goal may be to provide a strong material, but the structure may also result from quite different biological constraints. This implies that we may not succeed if we follow without modifications the solutions found by nature as optimal for a certain often unknown requirement. As a consequence, we have to carefully study the biological system and understand the structure-function relationship of the biological material in the context of its physical and biological constraints. Careful investigation of biological systems serving as the model is a prerequisite of biomimetic materials research

Research needs

The goal is to study the time-dependent changes in structure which enable one or several functions, such as photosynthesis, motility, color adaptation or strength and which are usually triggered by stimulus (light, electrical signal, thermal). This implies in-situ experiments in an environment as close as possible to the natural one.

Barriers

There is the need for very special specimen environments, problems with radiation damage during exposition to radiation, challenges concerning signal levels at high time and space resolution in spectroscopy, diffraction, imaging or tomography. Large data sets and high collection rates need an effort in software development. Due to the multi-disciplinary experimental approach, there is a special need for education.

2) Define new principles of materials design and synthesis

The mechanistic understanding of biological materials needs to be understood in a complete theoretical framework that allows extraction of abstract principles by which new materials can be designed, tailored and synthesized in a biomimetic way. The type of theoretical approaches will depend to a large extent on the function considered, such as quantum mechanics for photoelectric processes, finite element and analytical multiscale modelling for mechanical properties or statistical mechanics and network modeling for adaptation processes. A particular challenge is the fact that biological materials constructed and optimised on nearly all levels, from the molecular to the macroscopic dimensions. There is no size range in which biological materials can be considered homogenous. This complexity requires a well-organized experimental and theoretical platform enabling a true multi-scale approach .

Research needs

The goal is to model and predict material behaviour of known biological systems, define mechanistic material laws based on natural solutions, create software packages and data bases adapted to biological and biomimetic materials. Theoretical models need to be validated against natural systems, against artificial model systems, and against natural systems modified in their properties by chemical or molecular biological means (e.g. transgenic organisms). It is particularly important to numerically model and predict synchrotron and neutron data.

Barriers

Since all natural and most biomimetic materials are hierarchically structured, multi-scale analysis is needed from the molecular to the macroscopic level and over many time scales. A major challenge is the need for an integrated approach including theoretical modeling, structure and property determination, materials science and biology.

3) Develop new strategies for design, synthesis and processing of multifunctional materials based on bioinspiration

Nature has to synthesise materials under boundary conditions in temperature, pressure or time that may not be relevant for engineering; the solution for nature can usually not be simply extrapolated.

Research needs

The goal is to develop synthesis or processing routes leading to complex nanostructures, which are known from the analysis of natural systems to provide the right properties and multiple functions required for a given product. There is a need for online monitoring of synthesis and processing, using neutrons and synchrotron radiation, among other techniques.

Barriers

New synthesis and processing techniques need to be devised to reach the desired hierarchical structures, sometimes using base materials different from what natures herself does. The complexity of the structures to be made is a challenge.

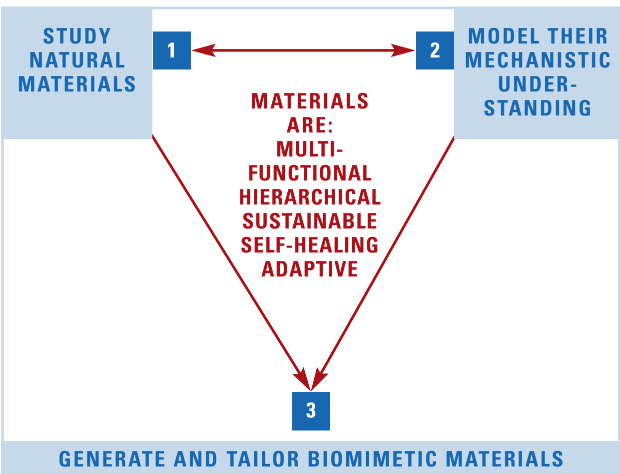


Fig. 3.5.20: Three major topics in biomimetic materials research. The circled numbers refer to the paragraphs in this section. In-situ characterisation techniques using neutrons and synchrotron radiation are needed at all three steps.

3.6. POLYMERS – SOFT MATTER: NANOSCIENCE AND NANOTECHNOLOGY

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Polymers are characterised by (weak) long-range intra- and intermolecular interactions leading to the formation of static and dynamic structures of hierarchical nature and physical-chemical properties depending on cooperative action at various length and time scales. The increasing knowledge about intermolecular interactions and the possible static and dynamic structures – dependent on the physical-chemical nature of the single polymer molecule – will lead to the design of new polymeric materials with a specific order and structure at different length scales. The key for polymer research is the tailoring of nanostructures for desired properties of bulk structural- and functional polymers with long-range order. Scattering and nanoscale imaging techniques involving synchrotron radiation and neutron sources are the most versatile and essential tools for this development. The spectrum of potential usages of polymers is given in the following diagramme (see Fig. 3.6.1).

Polymeric materials can be sub-divided into: i) structural polymers: emerging from large scale production and ii) functional polymers: used in very specific applications. Fig. 3.6.2. reviews the main groups and families of synthetic polymers and biopolymers.

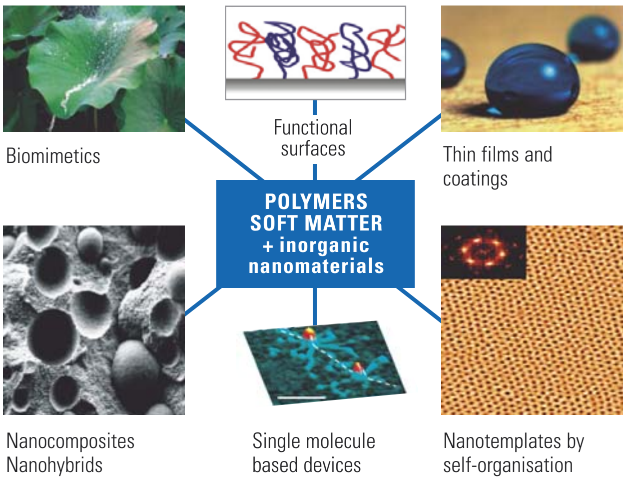

Fig. 3.6.1: The use of polymers in the design of nanomaterials.

3.6.1. POLYMERS IN BULK INDUSTRIAL PROCESSING CONDITIONS

Status:

Polymer science is a successful branch in soft condensed matter science with large-scale production and applications as bulk structural materials. In spite of the apparent successes, the solid, melt and solution states of classical polymeric materials are far from being understood and therefore will remain priority areas of "cutting-edge, innovative" research in order to be able to compete with US and Japanese industries. One should realise that, in European industry, the penetration of synchrotron radiation and neutron research in polymer science, has, until today, remained extremely weak.

Breakthroughs:

The ultimate macroscopic thermal, mechanical, optical and functional properties of polymer type materials are mostly realised for bulk samples by proper handling, involving melting, quenching, crystallisation, mechanical deformation, fibre formation, mixing with nanoparticles, and melt shearing. The result of the latter processing conditions is mostly studied post mortem. In all those fields, important breakthroughs will be made by exploring in-situ and in real-time the structural changes by preference at least at the millisecond level and lower. Structure sampling should be developed by simultaneous multi-scale approaches involving thermal (DSC), mechanical (deformation), optical (SALLS) analyses in conjunction with SAXS/WAXD. Synchrotron radiation is the tool of preference in this type of study.

BULK STRUCTURAL MATERIALS	FUNCTIONAL POLYMERS
Standard polymers: · Polyolefins · Engineering polymers · Copolymers · Polymer blends Biodegradable polymers and biopolymers: · Carbohydrate based biopolymers · Biopolymeric polyelectrolytes · Synthetic biodegradable polymers · Composite materials with bio-polymers Bulk multicomponent systems	· Multiblock copolymers · Conducting polymers · Polymers for photonic applications · Self-assembly based polymer-like materials · Polymer liquid crystals · Polymer-based sensors · Polymers for colloidal systems · Polymer-based supramolecular systems · Polymers for biomedical applications · Polymers for coatings · Polymers as adhesives

Fig. 3.6.2: Synthetic polymers and biopolymers.

3.6.2. FUNCTIONAL POLYMERS

Status:

In contrast with bulk applications of structural materials, interest arose in recent years to explore the potential of polymeric materials for applications in microelectronics, optical applications, biomimetic systems, intelligent pharma delivering devices, functional surfaces, displays, intelligent stimuli sensitive gels, etc. The first nanodevices have recently been developed and further progress in the development of diverse types of applications will greatly benefit from a joint European strategy.

Breakthroughs:

There are breakthroughs to be expected by developing tailor-made polymers concomitant with strong efforts to explore new synthetic pathways and new catalysts. Moreover, it is a new and recent finding that the behaviour of polymer chains in confined spaces is completely different from bulk behaviour. Hence, a completely new field of research has emerged which probes the nanostructures of synthetic polymers and biopolymers under confinement in: nanolayers, nano-multi-layers, nanodroplets, nanotubes, nanoporous systems and

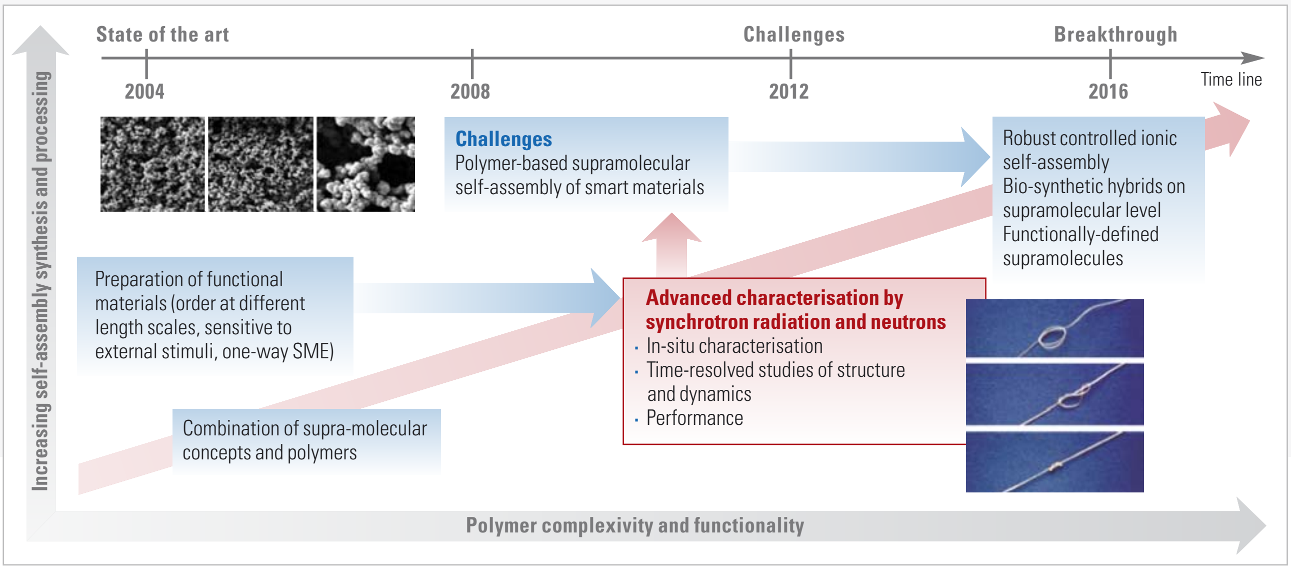

Fig. 3.6.3: Functional polymers: Roadmap for polymeric self-assembly based complex systems.

microfluidic systems. Such findings can then be implemented in the production of the following: protective coatings, reactive coatings, stimuli responsive coatings, adhesives, membranes for mimicking biological systems, and microfluidics. In addition, they can be used in technology (fuel cells), micelles and microemulsions, as well as in catalytic systems. Here again, synchrotron radiation and neutron scattering mediated research is crucial in exploring such systems because of their potential to probe the nanoscale structural features. Parallel to the developments in nanoscience and technology, new challenges appear to optimise synchrotron radiation and neutron scattering tools: improved optics, nanofocussing devices, manipulation of nanosized samples and a huge effort in counter development for synchrotron radiation and neutron scattering applications (see Fig. 3.6.3).

3.6.3. STRUCTURAL POLYMERS

Breakthroughs: Breakthroughs are to be expected in developing engineered polymers based on new synthetic methods, in order to upscale existing methods. Developments in advanced theory methods enable a detailed understanding of molecular conformation and structure, which can be probed by state-of-the-art synchrotron radiation and neutron experiments. This feeds through to an understanding of processing, leading to improved products for the consumer in the packaging and medical fields. Processing itself can be studied through in-situ scattering experiments. Structural polymers that are biodegradable or biocompatible will be of increasing interest – novel materials require synchrotron radiation and neutron characterisation, especially for in-situ measurements (see Fig. 3.6.4).

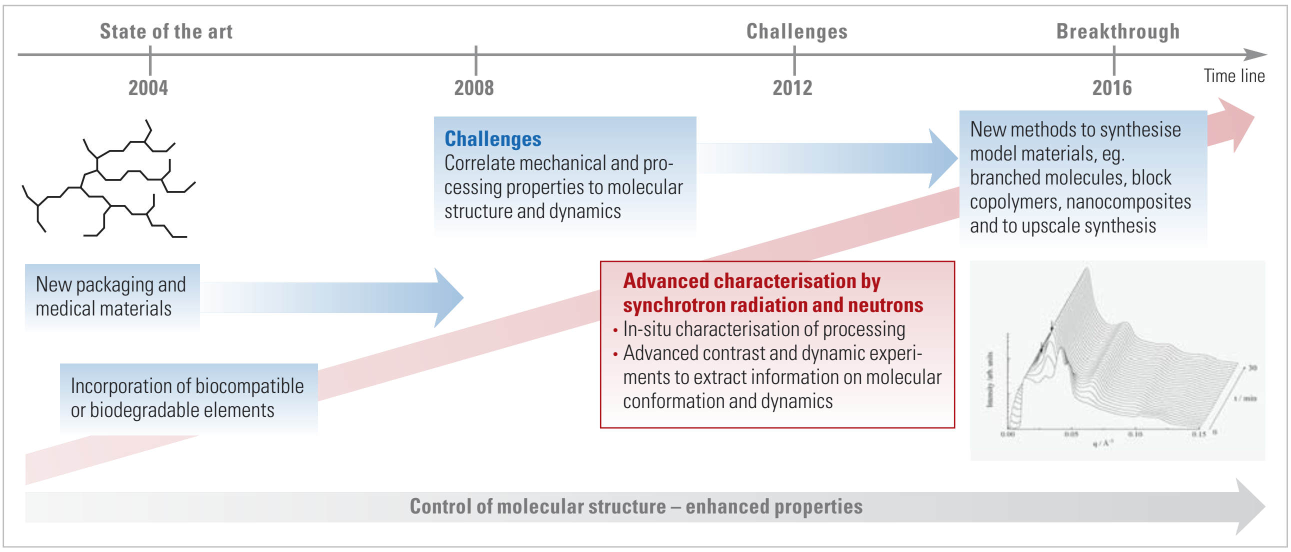

Fig. 3.6.4: Structural polymers: Roadmap for development and advanced characterisation of new bulk structural materials with superior properties.

3.6.4. POLYMERS: NANOSCIENCE AND NANOTECHNOLOGY – THE CHAIN OF KNOWLEDGE

POLYMER SYNTHESIS:

Aims: To create structural and functional polymer materials at low costs, under safe conditions and in an environmentally-friendly way; Rational design (computer-aided) with respect to predictability of chain microstructure and resulting structure-function relations.

New synthetic pathways:
- Catalysis
- Controlled-free radical polymerisation
- Polymerisation in nanostructures

Strict control of molecularity: Molar mass and polydispersity branching, tacticity, chirality, functionality

Breakthroughs:
- New polymers and block copolymers
- Highly pure polymers for medical, optical and electronic applications
- Self-assembly based nanostructures

TAILORING POLYMER PROPERTIES BY INDUCTION OF NANOSIZED STRUCTURES:

In polymer melts, in a mesophase, in the solid state, in confined space or in solvents. Towards new and improved properties of polymer materials.

- From polymer melts and mesophases towards polymer solids
- Polymers in solvents
- Nanostructured systems and polymers in confined space

FUTURE NEEDS FOR UNDERSTANDING AND STEERING OF NEW DEVELOPMENTS AND PRODUCTS:

Nanoscience
- Prenucleation
- Melt memory effects
- Mesophases

Nanoscience
- Fundamentals of polymer crystallisation

Nanoscience
- Polymer networks and gels

Nanoscience
- Influence of dimensionality and size constraints on polymer properties

Steering processing
- Extremely fast cooling
- Melts at HT and HP
- Melt orientation by flow
- Melts in HV/HF electric fields
- Chain dynamics in the melt
- Crystallisation at very low temperature
- Melts in strong magnetic fields

Producing order-disorder based bulk materials
- Templating crystallisation with nanoparticles and nanotubes
- Ultra strong fibres
- Nanowires
- Oriented films

Create intelligent gels
- Conformational gelation
- Kinetics of gelation
- Chain dynamics during gelation
- Intelligent stimuli responsive gels
- Complex gels involving nanoparticles

Structure in/of:
- Nanolayers
- Nanomultilayers
- Nanodroplets
- Nanoporous systems
- Nanotubes
- Microfluidics

3.6.5. BLOCK COPOLYMERS

Self-organisation of soft materials is a powerful route to the 'bottom-up' fabrication of nanostructures. The ability of soft materials such as block copolymers to form a rich variety of nanoscale periodic patterns offers the potential to create high-density arrays for use in data storage, electronics, molecular separation, combinatorial chemistry and DNA screening (see Fig. 3.6.5). Block copolymers exhibit a variety of bulk morphologies (depending on the ratio of block lengths, the segment-segment interaction parameter and polymerisation). Block copolymer thin films have a high application potential.

The length scale of microphase separation, 10–100 nm, is particularly interesting for future technologies based on a new generation of sub-micron scale electronic and optical devices. Such schemes would leverage the spontaneous self-assembly of these materials to create nanoscopic device components or templates. Tuning molecular parameters and microphase domains with a variety of motifs, chemistries, and tailored size and periodicity, a whole spectrum of block copolymer nanobased systems might be created. Current developments in block copolymer synthesis, such as atom transfer radical polymerisation, will widen the spectrum of available copolymer materials or decrease the manufacturing cost.

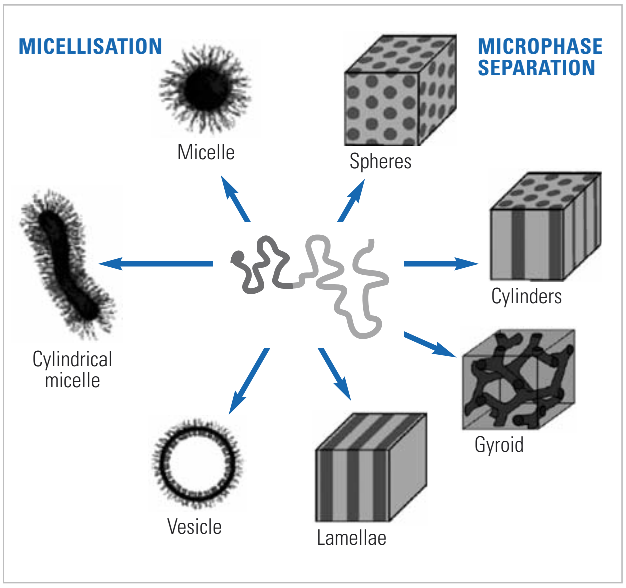

Fig. 3.6.5: Self-organisation structures of block copolymers.

Future developments will focus on:

- **Nanolithography**

Current photolithography produce feature sizes down to 100 nm, with strongly increasing manufacturing costs upon moving to shorter wavelengths. In semiconductor patterning using self-assembly, ordered (and oriented) layers of microphase domains, deposited onto a suitable substrate, are selectively etched to remove one of the block components. The resulting nanoholes allow replication of the block copolymer motif pattern onto the substrate (silicon, gallium, gallium arsenide, silicon nitride and oxide, alumina, magnetic materials). One promising application is the development of a self-assembly route for a high-density magnetic storage medium (cobalt nanodots).

- **Nanoporous materials**

Selective removal of block copolymer film domains carries the potential for the formation of nanoporous membranes with well defined channel sizes and pore sizes tailored through the block copolymer composition and molecular weight.

- **Nanoparticle patterning at surfaces**

Nanoparticles at surfaces can be patterned using the self-organisation of block copolymers. Metals, metal oxides and alloys, ceramics, electro conductive polymers, semiconductors and carbon nanotubes can be deposited by physical- or chemical vapour deposition techniques with so-called decoration effects in the case of PVD or CVD.

- **Nanoreactors for nanoparticle production**

Block copolymer domains are future 'nanoreactors' for the synthesis of inorganic nanoparticles by the binding of inorganic species to the monomer prior to polymerisation or by ion binding the blocks of a copolymer prior to micellisation. A further promising concept involves the loading of pre-formed micelles (in solution or in bulk). A variety of metal nanoclusters have successfully been templated within block copolymer domains in this way.

- **Nanocapsules**

Future strategies include vesicles formed by block copolymers in solution for the synthesis of hollow nanoparticles with a polymeric shell. Nanocapsules ('polymersomes') can be prepared using appropriate diblocks, which exhibit enhanced toughness and reduced water permeability. Nanocapsules with a cross-linked diblock shell have a great potential for drug delivery. Additional advantages are the enhanced stability (for example in the bloodstream) and the ability to tune the capsule size and to incorporate responsive and/or functional moieties.

- **Photonic crystals**

The self-assembled morphologies of block copolymer systems that spontaneously exhibit well-defined alternating layered structures make them intriguing candidates for photonic applications.

Key challenges

- Tailoring the photonic layer period by addition of homo-polymers;
- Tailoring their index of refraction by selective doping with high-index particles;
- Synthesis of bio-inspired nanostructures templated by peptide-based copolymers;
- Synthesis of morphologies with hierarchical ordering;
- Block copolymers in confined space.

Future role of synchrotron radiation and neutrons

- Synchrotron radiation will be of particular interest for the study of nanostructured block copolymers with nanomaterials, especially for the in-situ monitoring of aggregation during melt compounding ("Rheo-SAXS").
- Synchrotron radiation experiments using microfocus beams allow microscopic information with high spatial resolution.
- Future x-ray nanobeams will allow access to the space distribution

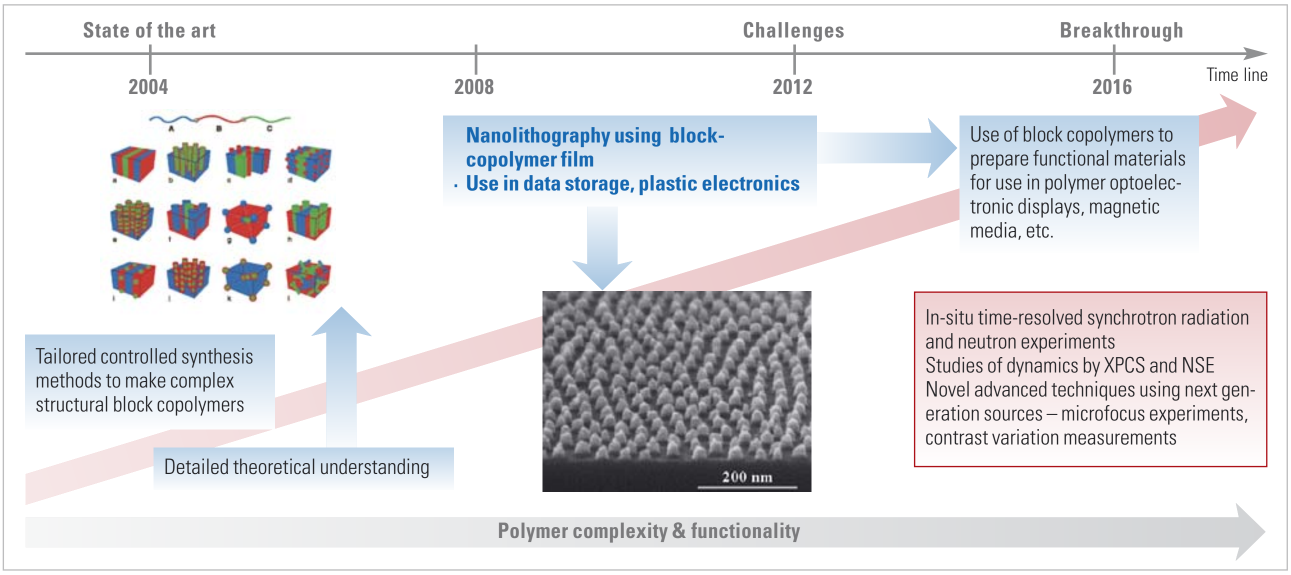

Fig. 3.6.6: Roadmap highlighting new synchrotron radiation and neutron techniques and methods for the study of block copolymers.

of the nanophase in the polymer medium and to the structure identification of nanofibres
- Dedicated x-ray tomography beam lines with high spatial resolution are of utmost importance in the study of nanostructured block copolymers.
- Stroboscopic x-ray photon correlation spectroscopy (XPCS) in the MHz regime must be developed to such a reliable state to allow measuring the dynamic properties of nanopolymeric materials, 'hairy' magnetic nanoparticles and electrically charged nanoparticles.
- Neutron spin echo (NSE) spectroscopy is most important for the microscopic understanding of the dynamics of block-copolymers
- In combination with deuteration, neutron spectroscopy techniques provide the unique possibility to tag specific components and to determine chain conformations of macromolecules.
- Thin film nanostructures, grazing incidence scattering and reflectivity. In-situ measurements during spin coating.

A roadmap for block-copolymers research using synchrotron radiation and neutrons is schematically given in Fig. 3.6.6.

3.6.6. POLYMER NANOCOMPOSITES

Polymer nanocomposites are a class of reinforced polymers with low quantities of nanosized inorganic (mainly plate-like, spherical or cylindrical) ingredients. The spatial self-organisation between the incompatible components leads to novel structural features, physical-chemical properties, and complex functions. The main applications are automobile, construction, electronic and food packaging technologies (see Fig. 3.6.7 and Fig. 3.6.8).

Future challenges and breakthroughs

- Polymer nanocomposites with incorporated metal oxide clusters are only beginning to show their potential as an interesting new class

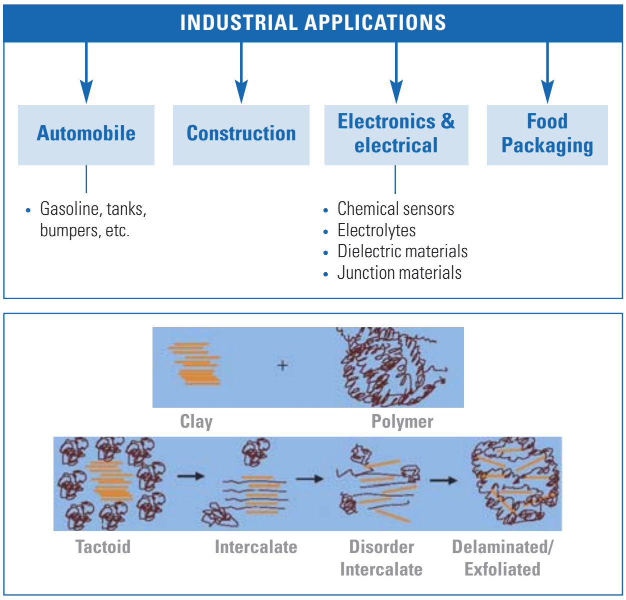

Fig. 3.6.7: Industrial application of polymer nanocomposites.

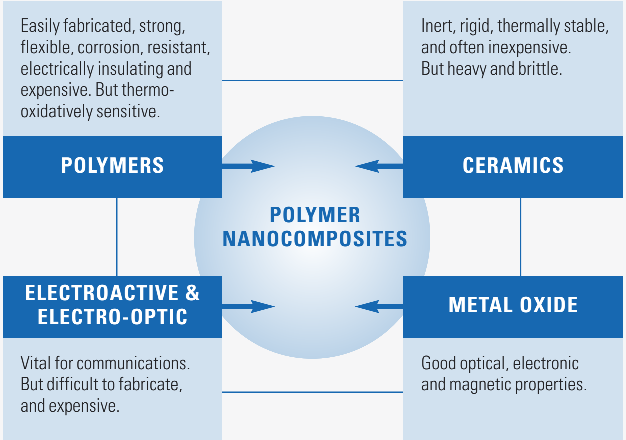

Fig. 3.6.8: Illustration showing the components of polymer nanocomposites.

of inorganic-organic hybrid polymers, which may exhibit interesting optical (planar wave guides), electronic and magnetic properties. Substantial improvements are mandatory in the thermal stability and in their use in patterning by photolithography or reactive ion etching.

- Nanocomposites based on conducting polymers and transition metal oxides have a strong potential as active components in lithium batteries and as optoelectronic devices. The magnetic metal oxide-polymer nanocomposites have a great potential in device technologies for high density memory and magnetic recording applications. However, a significant improvement of magnetic properties (super-paramagnetic behaviour at room temperature and ferri-magnetic behaviour at low temperature) by self-assembly of the magnetic nanoparticles or other induced order inside the polymer matrix is a necessary prerequisite.

- Organic-inorganic nanocomposites have a huge potential in electronics and optoelectronics, including light-emitting diodes, photodiodes, solar cells, gas sensors and field effect transistors. Several hybrid polymer solar cells have been reported by combining conjugated polymers with n-type inorganic semiconductor nanoparticles such as CdSe, TiO_2 and ZnO. Despite the progress made in this field, polymer photovoltaics are still in its early infancy. Up to now, the power conversion efficiency of the devices is rather low (less than 4%), and the stability is not very good. Even with proper protection, there are several degradation processes that need to be eliminated to improve stability.

The main issues of future research include a further understanding of operation phenomena (interfaces, charge transport, morphology control) and degradation of these cells. This will lead to much higher power conversion efficiencies and lifetimes that are sufficiently long for practical use. It is expected that, in the future, it will be possible to construct high-performance and low-cost field-effect transistors by fabricating ideal organic/inorganic interfaces.

Future role of synchrotron radiation and neutron facilities

The main question concerning the improvement of nanocomposites is to understand how structural changes and physical properties are interrelated (see Fig. 3.6.9).

Systematic structural x-ray and neutron investigations have to be carried out to elucidate the structural properties at very different length scales. Particular important structural features and phenomena are:

- The correlation length of the fractal aggregates and the fractal dimension;
- The mesoscopic structure;
- The secondary supermolecular aggregation;
- The organic-inorganic interactions and particle distribution;
- The isothermal crystallisation rates and its connection to the crystallinity and crystallisation type of polymers in nanocomposites;
- The chemical composition of surfaces.

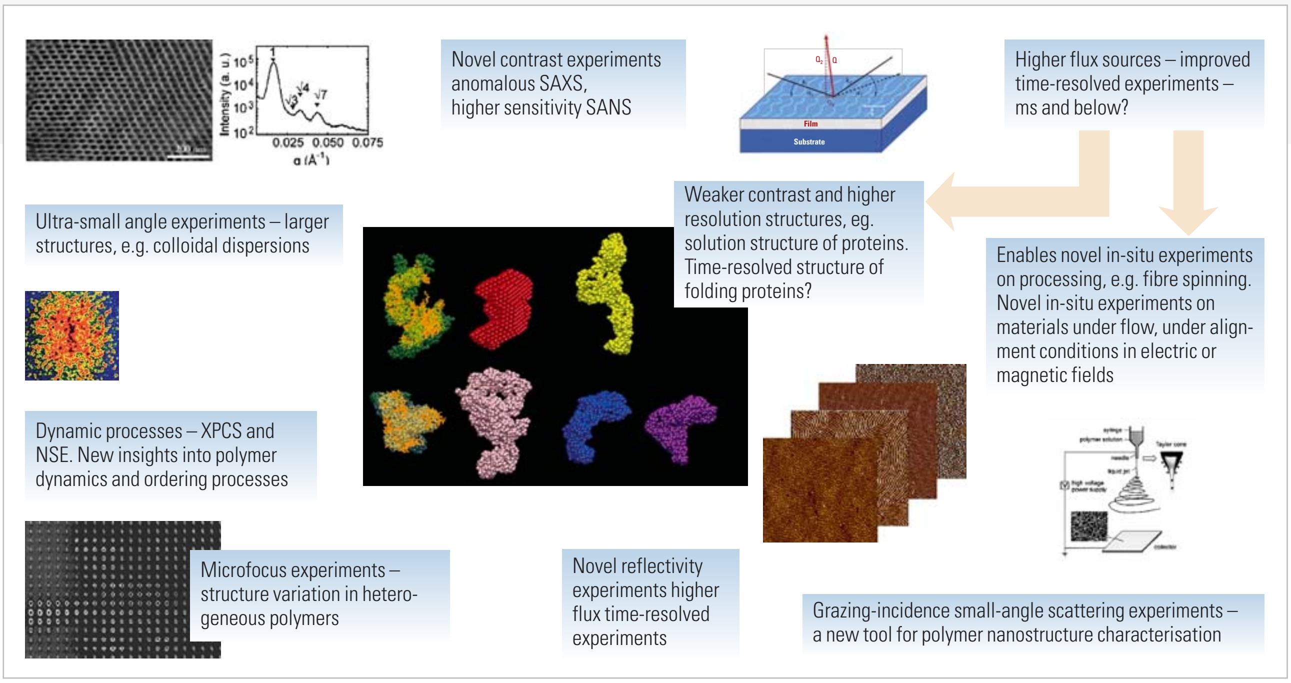

Fig. 3.6.9: Roadmap for new synchrotron radiation and neutron techniques and methods mediated for polymer research.

ACTIONS FOR POLYMER NANOSCIENCE AND NANOTECHNOLOGY

GRAND CHALLENGES
Structural polymers:
- Tailoring properties based on understanding of molecular structure and dynamics, model materials, e.g. branched polymers
- Build on European world-leading expertise in this field

GRAND CHALLENGES
Biodegradable/biocompatible polymers:
- Packaging materials
- Renewable resources
- Environmentally-friendly

SYNCHROTRON RADIATION AND

GENNESYS SOFT MATTER CENTRE

NEUTRON FACILITIES

GRAND CHALLENGES
Biopolymers:
- Protein folding – peptide fibrillisation
- Development of biopolymers from renewable resources
- Biomimetic materials
- Tissue scaffolds, drug delivery systems

GRAND CHALLENGES
Functional polymers:
- Novel opto electronic polymers for displays, sensors
- Functional polymers for biomedical applications
- Relevance to IT, communications, medical industries

Fig. 3.6.10: Roadmap highlighting new synchrotron radiation and neutron techniques and methods for the study of block copolymers.

3.6.7. CONCLUSIONS AND RECOMMENDATION

Future role of synchrotron radiation and neutrons for polymer research

Experiments

- In-situ time-resolved nanomaterials science under industrial processing conditions;
- Investigations involving simultaneous SAXS and WAXD;
- X-ray imaging and tomography;
- Study of radiation damage (SR).

Beam lines

- Dedicated beamlines for: USAXS/USANS;
- Nanofocussing and nanosized beams;
- X-ray photon correlation spectroscopy;
- Neutron spin echo spectroscopy.

New experimental developments for research involving

- Very high magnetic fields;
- High pressures;
- High voltage electric fields;
- Controlled fast heating and cooling.

Equipments

- Fast read-out electronics for detectors;
- Detectors with improved spatial resolution;
- Improved support for deuteration.

Research policy requirements

- Continuous development of x-ray optics, optimising the performance of counting devices, and realisation of the 'ultimate storage ring' and the European Spallation Source;
- The use of synchrotron radiation and neutrons needs to penetrate all aspects of structure-function relation studies in soft condensed matter and especially in polymer science oriented industries;
- Stimulation of young scientists to explore and develop the full potential of the synchrotron radiation and neutrons approach in the framework of nanoscience and nanotechnology-oriented doctoral research projects with at least a one year commitment at synchrotron radiation and neutrons sources;
- Facilitate the implementation of synchrotron radiation and neutron mediated nanoscience and nanotechnology in industry by creating an interface between academic science and industrial technology: an European GENNESYS research centre for soft condensed matter;
- Increase the number of temporary post-doctoral positions at synchrotron radiation and neutrons facilities;
- Create part-time GENNESYS professorships for leading scientists.
- Mobility of researchers across Europe, between distributed GENNESYS nodes;
- Build high flux European neutron source.

3.7. INORGANIC NANOMATERIALS

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3.7.1. INORGANIC NANOPARTICLES AND ORGANIC-INORGANIC NANOCOMPOSITES

Research on inorganic nanoparticles and organic-inorganic nanocomposites not only includes synthetic work, but also the characterisation of the structural, chemical and physical properties, assembly into 1-, 2- and 3-dimensional superstructures extending over several lengths scales – potentially with hierarchical architectures, and application in various fields of technology. However, most of the research efforts are still dedicated to the development of new synthesis routes. It is without a doubt that the in-depth investigation of the physical and chemical properties represents a key step on the way to a faster implementation of inorganic nanomaterials into technological applications, and thus has to be intensified.

State of the art: research

The large number of synthesis techniques developed in the last decades gave access to inorganic nanomaterials with a wide range of compositions, well-defined and uniform crystallite sizes, extraordinary and unprecedented crystallite shapes, and complex assembly properties. The synthesis methods can basically be divided into liquid-phase routes and gas-phase processes (Fig. 3.7.1). In gas-phase processes (Fig. 3.7.1, right-hand side), nanoparticle formation can either be driven by chemical reactions of gaseous precursors (chemical routes) or by cooling a vapour (physical routes): chemical routes are processes driven by hot-wall tubular furnaces, flames, plasmas, and lasers. Physical processes typically involve the cooling of a hot vapour, produced by different heating techniques (laser ablation, sputtering), by expansion, by mixing with a cooler gas, or by heat transfer to the surroundings using, for example, a nozzle, a free convective plume or an electrospray system. Liquid-phase routes (Fig. 3.7.1, left-hand side) include coprecipitation, hydrolytic as well as nonhydrolytic sol-gel processes, microemulsions, hydrothermal or solvothermal methods, biomimetic approaches, and template synthesis. However, often the synthesis protocol for a particular nanomaterial involves not just one, but a combination of several of these methods.

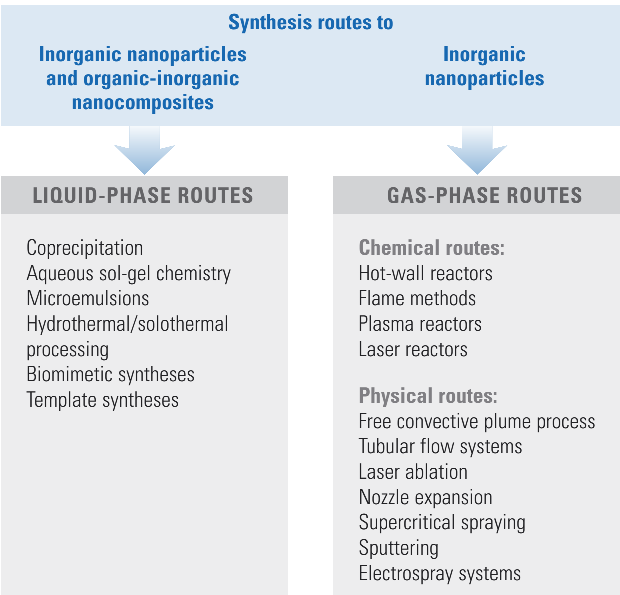

Fig. 3.7.1: Overview of synthesis routes to inorganic nanoparticles and organic-inorganic nanocomposites via liquid-phase and gas-phase methods.

Gas-phase and liquid-phase routes are rather complementary and both approaches have advantages and limitations. Table 3.7.1 summarises the pros and cons of the two strategies. It should be kept in mind that this list merely reflects some general trends.

	GAS-PHASE ROUTES	LIQUID-PHASE ROUTES
Pros	· High purity · Excellent scalability · Low cost · Direct fabrication of powders or films (dense or porous) · Good reproducibility · High crystallinity	· Simple equipment · Low temperature · Control over surface properties/ functionalisation · Good redispersibility · Synthesis of organic-inorganic nanocomposites possible · Small particle size distribution possible ($\sigma < 5$ %) · Large variety of shapes · Multi-metal and doped compounds accessible
Cons	· High temperature · Aggregation/agglomeration · Surface functionalisation with organic groups not yet possible · Organic-inorganic nano-composites not accessible · Multi-metal compounds hardly accessible	· High price · Contamination from solvent/ additives · Bad scalability · Sensitive to slight variations in synthesis conditions

Table 3.7.1: Pros and cons of gas-phase and liquid-phase routes to inorganic nanoparticles and organic-inorganic nanocomposites.

Future research needs

Although the synthesis of inorganic nanoparticles and organic-inorganic nanocomposites made immense progress in the last few years, there are still a lot of open questions in the broad field of nanoparticle research. Some of the future challenges are summarized in Fig. 3.7.2.

Whereas some of these topics have already been the focus of intense research for several years, other problems and questions have just recently become of interest to the scientific community. Fig. 3.7.2 divides research on inorganic nanoparticles and organic-inorganic nanocomposites into six sub-topics:

Synthesis

- Control over composition, size, size distribution, shape, and crystal structure;
- Synthesis of multi-metal and doped nanoparticles (e. g. superconductors, manganites);
- Synthesis of nanoheterostructures containing sections of compositionally different inorganic materials;

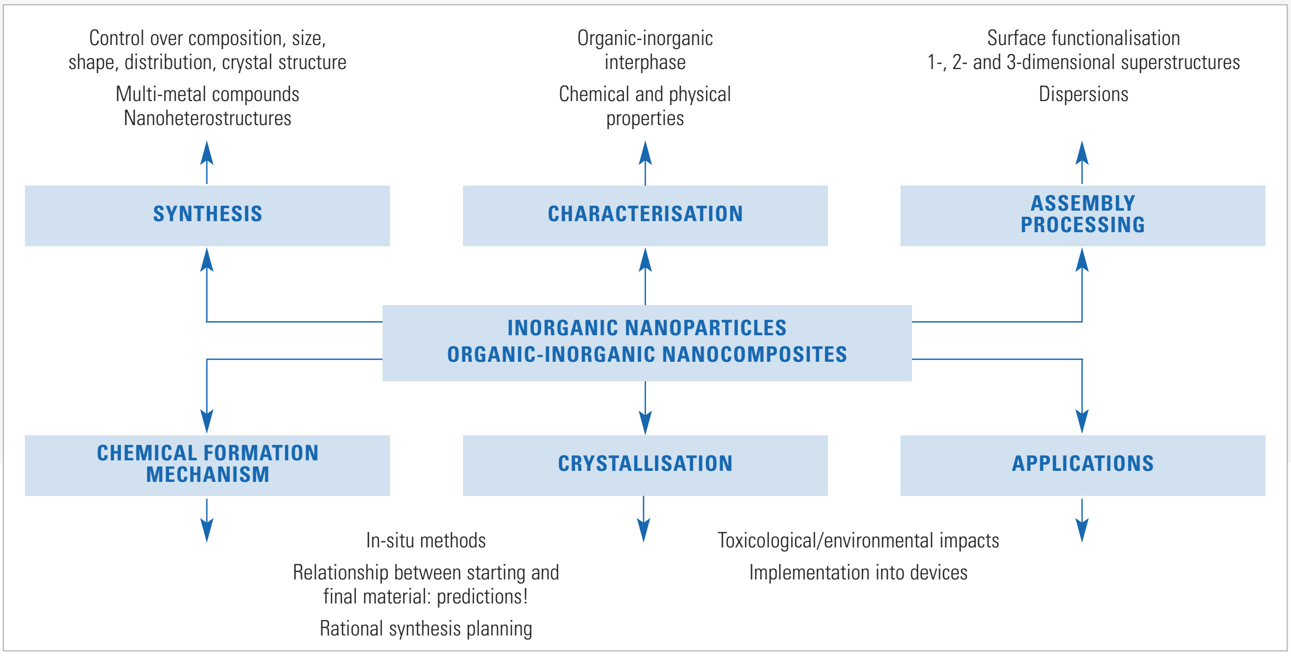

Fig. 3.7.2: Major challenges in the research area of inorganic nanoparticles and organic-inorganic nanocomposites.

- Synthesis of organic-inorganic nanocomposites (new combinations of organic-inorganic components with a similarly strong focus on the functionality of the organic part);
- Synthesis of "new" classes of materials on the nanoscale: metal nitrides, metal carbides, alloys, zintl phases;
- "Greener" synthesis procedures;
- Rational synthesis planning/predictions.

Characterisation

- Structural characterisation beyond common laboratory techniques (e.g. synchrotron x-ray diffraction and neutron scattering for the study of poorly crystalline nanomaterials and local structural order, neutron scattering for the determination of magnetic structures and spin dynamics);
- Characterisation of the organic-inorganic interphase (on the surface of the nanoparticles as well as within the organic-inorganic composites);
- Study of the chemical and physical properties;
- Development of new characterisation tools with ever finer resolution.

Assembly and processing

- Surface functionalisation to control the agglomeration and assembly properties, as well as to tailor binding affinities towards other surfaces/particles and molecules;
- Use of nanoparticles as building blocks for the fabrication of 1-, 2-, and 3-dimensional, possibly hierarchical, architectures over several length scales;
- Controlled patterning/deposition of nanoparticles;
- Direct processing of nanoparticles into bulk materials (thin films, ceramics, coatings, electrodes, sensors, catalysts);
- Production of nanoparticle dispersions (with high solid content).

Chemical formation mechanisms

- In-situ studies during synthesis (e.g. neutron scattering for the study of dynamical phenomena);
- Characterisation of all species initially present and in-situ formed during synthesis;
- Elucidation of the chemical role of the different species in solution on a molecular level at all stages of nanoparticle growth;
- Correlation between synthesis system [precursor(s) and solvent(s)] and final composition and surface properties.

Crystallisation mechanism

- Study of the liquid-solid interphase during all stages of crystallisation;
- In-situ study of the crystallisation process (e.g. neutron diffraction in real time under genuine reaction conditions, EXAFS (extended x-ray absorption fine structure) and EDXRD (energy-dispersive x-ray diffraction) investigations for the study of crystallisation kinetics…);
- Correlation between synthesis system [precursor(s) and solvent(s)] and final morphological (size, shape, size distribution) and structural (crystal structure) characteristics;
- Modelling.

Applications

- Study of health, safety, and environmental aspects (including potential long-term effects);

- Implementation into (nano-)devices, potentially resulting in one-particle devices;
- Combination with other classes of nano- and bulk materials (composites, hybrids);
- Stability of nanostructured materials during operation (e.g. thermal, chemical, and structural (long-term) stability);
- Scalability, reproducibility and cost-effective production;
- See also "Assembly and processing".

The main challenge of nanoparticle research clearly lies in the development of synthesis concepts based on a rational strategy. It is still impossible to prepare a certain compound on the nanoscale with a desired composition, structure, size and shape, or even properties, intentionally and in a predicted way. The main reasons for this major limitation can be found in the poorly understood crystallisation mechanism of nanoparticles and organic-inorganic nanocomposites, as well as in the hardly investigated chemical formation pathways involved in the formation of inorganic nanomaterials. Most notably, the liquid-solid (or gas-solid) interphase during the growth of inorganic nanomaterials is not yet understood on a molecular level. It will be absolutely essential to strengthen the use of in-situ methods for the study of nanoparticle growth under experimental conditions.

Importance of synchrotron radiation and neutrons in future research and development

In order to advance with the rational design of new materials, synchrotron radiation and neutron based methods are key techniques. They will not only allow insight into the structure-property function relationships, but will also allow investigate, and the first entities formed in a solution or in the gas phase before the solid material forms. Future efforts should not only focus on improving the methods behind the experiment (higher intensity, higher brilliance for spatial resolution, new element sensitive techniques) but also the design of sophisticated in-situ cells. This allows a combination of synthetic procedures from the lab with characterisation of the materials by x-ray or neutron based techniques.

As shown in Fig. 3.7.1, many of the processes occur in the liquid phase. Here, the role of spectroscopy is the identification of small entities and clusters in the first stages. Scattering and x-ray absorption or fluorescence techniques are excellently suited for this type of identification, but the kinetic identification requires high incoming x-ray intensities. Using stopped flow techniques, highly focussed beams available at the newest synchrotrons appear important, including those which are presently in the planning phase. Not just highly focussed x-rays but also infrared radiation is of interest. Once more crystalline structures are formed, the components can be identified by complementary diffraction techniques. This shows the importance of both advanced multi-spectroscopic tools (which provide the complementary information) and time-resolved methods. The latter can give insight into the kinetics and possible intermediates that may determine the final structure. This information can hardly be obtained by laboratory techniques alone and both neutrons and x-rays offer the possibility to imitate the lab process.

Gas phase, supercritical and related routes can also be investigated in a related manner from the growth of the first clusters to the full functional nanoparticle. Almost as important as the nanoparticle formation itself, is its functionalisation. In certain cases surfaces are functionalised. In that case, grazing incidence and other surface sensitive techniques, preferentially performed under realistic process conditions, appear important. These investigations equally require both conventional and highly advanced sources. "Conventional" because the lab technique has to be combined with the experimental technique. Advanced sources are named as such because in certain cases high intensity and/or high brilliance are required. The ultimate goal is to come significantly below the 100 nm limit, since most processes and properties are determined on an atomic scale.

- High intensity for rapid kinetic studies;
- Complementary techniques to obtain information on short range order (molecular entities, clusters, amorphous materials) and long range order (crystalline materials);
- Spatial resolution for stop-flow experiments and in case of heterogeneous samples;
- Robotic-control at end stations for high throughput screening and effective beamtime use;
- Rapid scanning techniques and detectors for dynamic changes in the ms-scale.

3.7.2. MOLECULAR, INORGANIC MATERIALS AND HYDRIDES

The bottom-up approach is now well developed for nanofabrication and nanomanipulation procedures used in physics and materials sciences. It starts from the ultimate limit – or in other words from the atomic scale – to design and fully prepare new materials from "soft" chemical reactions, thus opening the route to scales unexplored until now. The building of objects in a "step-by-step" manner, by capturing the relationship between structure/properties in view of optical applications (sensors, displays, guides, photonic crystals, etc.), magnetism, catalysis and photocatalysis, phase separations (nanomembranes), or even vectorisation (specific encapsulation), seemed to be out of reach a decade ago. However, the development of new tools and synthesis protocols has introduced new and interesting perspectives in this field. This is crucial for the design of individual objects or even systems – showing self-organisation – that exhibit remarkable physical-, chemical- and biological properties. It includes several methods of preparation, such as the use of inversed micelles, sol-gel techniques, evaporation on surfaces, soft chemistry, supramolecular chemistry, and self-organisation processes (see Fig. 3.7.3).

Nanostructures and nanomaterials may be divided into two large classes:

i) Nanometric-sized objects (molecules, clusters, aggregates, wires, etc.), which are isolated or organised into networks;
ii) Nano- or mesoporous crystallised materials, which exhibit a network of tunnels or cavities obtained by molecular templating (molecular clusters, metals and metallic oxides, chalcogenides and III-V and II-VI semiconductors, fullerenes, as well as carbon nanotubes).

Materials offer properties (electronic, magnetic, optical, chemical, etc.) that differ from volume properties, and which offer numerous application capabilities. Aluminosilicates from alkaline metals or alkaline earth metals (zeolites) and metallophosphates, have been the object of numerous studies on the role of structuring agents (organic or inorganic species) in harnessing the size and shape of pores. These studies have been extended to porous solids with hybrid frameworks, involving strong binding between organic and inorganic species, which can also be synthesised by using molecular templates.

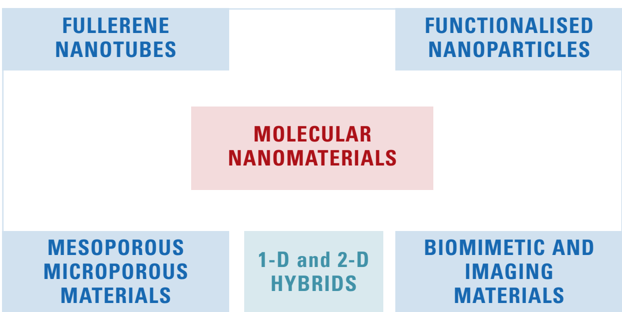

Fig. 3.7.3: Overview of molecular- and nanoinorganic materials.

The organisation of nano-objects on surfaces or in porous structures remains in the exploratory stage, despite the fundamental and applied applications for such systems. One of the promising approaches is the design of molecular precursor nanostructures that are associated with hybrid structures (objects on/in a semiconductor, inorganic, etc.), as well as the study of the parameters that govern the magnetic, optical or transport properties.

State of the art research

a) Chemical composition
- Compounds with multinary composition;
- Synthesis of highly-reactive/sensitive compounds (e.g. sensitive towards moisture, oxygen, temperature, ambient light) on the nanoscale;
- Selective doping of materials;
- Control of defect concentration and type of defects;
- Advanced composite materials and structures.

b) Morphology, shape and assembly
- Monodispersed, non-agglomerated spheres;
- Cubes, plates, needles, rods, etc.;
- Hollow structures, including hollow spheres, tubes etc.;
- Random packing, porous structures;
- One and two-dimensional assembly of nanomaterials;
- Three-dimensional close packing of nanostructures, photonic crystals, superlattices;
- Biomimetic control and growth, self-assembly.

c) Surface modification and surface conditioning
- Controlling and steering of size, size distribution, aggregate formation and morphology;
- Controlling and steering of materials transport, deposition and assembly;
- Core-shell structures, multiwall/multilayer structures;
- Organic-inorganic composites;
- Biocompatible surfaces.

d) Material properties and application
- Coating of macroscopic substrates or embedding in substrates (e.g. glass, paper, plastics) with nanomaterials for reasons of colouring, labelling, hardening, increasing scratch resistivity, UV-stabilisation, matching of refraction, wave-guiding, etc.;
- Electron conductivity and transparent conductive oxides;
- Fast ion conductors, including fuel cell applications or supercaps;
- Magnetism, including superparamagnetism, magnetic pigments;
- Luminescent materials (e.g. for displays, lamps, LED's, x-ray, two-photon processes);
- Thermal properties and thermoelectric effects;
- Mechanical properties, including piezoelectrics, actuators etc.;
- Catalysis;
- Specific surface, porosity of materials; adsorption of atoms/molecules;

- Quantum effects, including novel compounds showing quantum effects and novel types of quantum effects;
- Contrast agents, markers, labelling for biomedical purposes;
- Optical absorption/reflection, aiming at colour pigments, reflective pigments, wave-guiding, etc.

Overview of potential inorganic nanomaterials

Inorganic materials

- Nanoparticles of many types and shapes: i.e. nanocomposites,... etc.;
- Nanoporous minerals beyond Aluminosilicate zeolites: Aluminosilicate and phosphates $AlPO_4$s (hydroxyapatite, talc, spinels, transition metals and other phosphates);
- Metal sulfates, oxides, chalcogenides, halides, nitrides;
- Wide band gap oxides metal nanoparticles: i.e. Au, Ag, Al, Si, Pd, Pt, TiO_2, SiO_2, CeO_2, Fe_2O_3, and Fe_3O_4...;
- Ceramics: BN, Al_2O_3, SiC, Al_4C_3...;
- Semiconductors: GaN, ZnO, CdSe...;
- Various other inorganics: i.e. $BaCO_3$, $LnPO_4$, MS_2 (M=Mo,W, Nb etc.)

Many inorganic materials form open-framework polymorphs, but not all can be rendered nanoporous!

Organic materials

- Organic nanoparticles, such as dendrimers;
- Block copolymers;
- Molecular electronics, e.g. OLED's.

Potential applications

a) Buckyballs and carbon nanotubes

Structural materials, as in carbon nanotube reinforced composites:

- Sensors;
- Displays using Field Emission;
- Carbon nanotube transistors for molecular computers;
- Data storage;
- Hydrogen storage in carbon nanotubes for fuel cells;
- Photovoltaic cells;
- Scanning probe tips for AFM's;
- Water purification.

b) Inorganic nanoparticles

- Nanocrystals of gold functionalised with DNA for biorecognition;
- Platinum group metal nanorods for i.e. security barcodes;
- Nanocrystals of aluminium i.e. rocket propellants;
- Magnetic nanoparticles of iron for i.e. drug delivery
- Purification filters based on Al_2O_3 nanowires;
- Porous nanoparticles of silica for i.e. delivery of functional molecules;
- Nanocrystals of ZnO or TiO_2 for i.e. UV-absorption;
- Nanocrystals of zeolites and other materials for i.e. catalysis;
- MoS_2 onions for i.e. lubrication;
- Nanocrystals of CdSe, Si and TiO_2 for i.e. solar cells;
- Nanocrystals of SiC for i.e. ceramic applications;
- Calcium phosphate nanoparticles for i.e. bone applications;
- Nanoparticles of rare-earth phosphors for i.e. security tagging and solid state lighting;
- Nanoparticles of minerals for i.e. composites.

c) Organic nanomaterials

There is a wide range of organic and polymer nanoparticles that are finding applications in:

- Drug delivery, cosmetics, foods, catalysis, etc;
- Micelles;
- Liposomes;
- Dendrimers;
- Nanoemulsions;
- Calixarenes;
- Cyclodextrins.

d) Hybrid inorganic-organic materials

Coordination polymers with giant pore structures (> 60 %): i.e. Zn_4O (1, 4 benzenedicarboxylate): some of the lowest density materials (~0.1.m/ml) ever synthesised with remarkable surface areas (> 5000 m^2/g); using room temperature solvent routes. The structure may be tuned by adjusting sizes of linkers and modified by varying the carboxylic acids. They have the ability to adsorb very large molecules, e.g. peptides etc. and other guest molecules.

Conventional polymers: Ferroelectrics, ferroics;
Proteins: DNA, RNA High Tc superconductors;
Micelles, dendrimers: Colossal magneto resistance;
Emulsions, liposomes: Battery cathodes/anodes;
Molecular electronics: Quantum dots, phosphors;
Conducting polymers: Zeolites, clays;
Nanotubules: Electronic materials, II-V semiconductors;
Surfactants, phospholipids: Carbon nanotubes, buckeyballs.

Major materials trends in molecular, inorganic nanomaterials and hybrids – future research needs

a) Chemical synthesis

- Synthesis of nanomaterials, which are not yet available on the nanoscale (e.g. less-noble metals, alloys, halogenides, compounds with multinary composition);
- Choice and control of type, concentration and location of defects and dopants;
- Realise advanced composite nanostructures;
- Novel concepts of synthesis aiming at high reproducibility, yield and adaptability;
- Adjust highly adaptable strategies for surface conditioning independent from the conditions of materials synthesis.

b) Morphology and shape

- Steer and control size and shape of nanomaterials (e.g. size control with ±5 nm on full nanometre scale, 1–100 nm);
- Adjust shape (such as sphere, plate, needle, cube, rod, tube, etc.) for each specific compound/material;
- Tune size and shape by external forces (electrical, magnetical field, etc.);
- Biomimetric strategies to control and steer size/shape.

c) Superstructures and composite materials

- Use of advanced composite materials for optimised combination of properties;
- Develop general procedures to precipitate, assemble and structure nanomaterials, including one- and two-dimensional assembly of rods/tubes;
- Develop general strategies for bottom-up growth of superlattices, preferably with building units exhibiting different compositions, sizes or morphologies;
- Establish techniques to gain hierarchical or fractal structures;
- Explore and use bio-inspired materials and methods of synthesis.

d) Materials properties

- Modify and adjust material properties by variation of size and shape;
- Adjust material-structure-property relations;
- Establish theoretical calculation/prediction of material-structure-property relations;
- Controlled switching of properties, for instance, conducting/insulating, reflecting/transmitting, magnetic/non-magnetic, colour change etc.;
- Develop novel nanomaterials/-structures driven by means of application;
- Explore novel applications/techniques based on entirely new materials/composites.

e) Analytical characterisation

- Analyse type, concentration and location of defects and dopants;
- Develop advanced in-situ characterisation of nanomaterials, e.g. in biological systems, composites;
- Differentiate properties related to inner core and surface;
- Analyse diffusion and transport at grain boundaries;
- Three-dimensional imaging of nanomaterials/-structures (e.g. holographic methods);
- Analyse material properties (optical, electrical, magnetical) on a near atomic regime.

Role of synchrotron radiation and neutrons in the future research breakthroughs in inorganic nanomaterials

a) Materials composition

- Analyse concentration and location of defects in nanomaterials/-structures;
- Analyse concentration and location of dopants in nanomaterials/-structures;
- Analyse concentration and location of grain boundaries in particles;
- Differentiate different crystalline grains inside individual nanoparticles;
- Establish chemical analysis in the nanometre regime;
- Correlate materials composition and materials properties on a (near) atomic scale;
- Explore the magnetic properties of thin films built with these nanomaterials, especially using XMCD technique.

b) Diffusion processes

- Differentiate between core and surface allocated diffusion processes as well as electron and ion transport inside nanoparticles;
- Differentiate diffusion processes on different timescales (e.g., ns to min).

Research roadmap

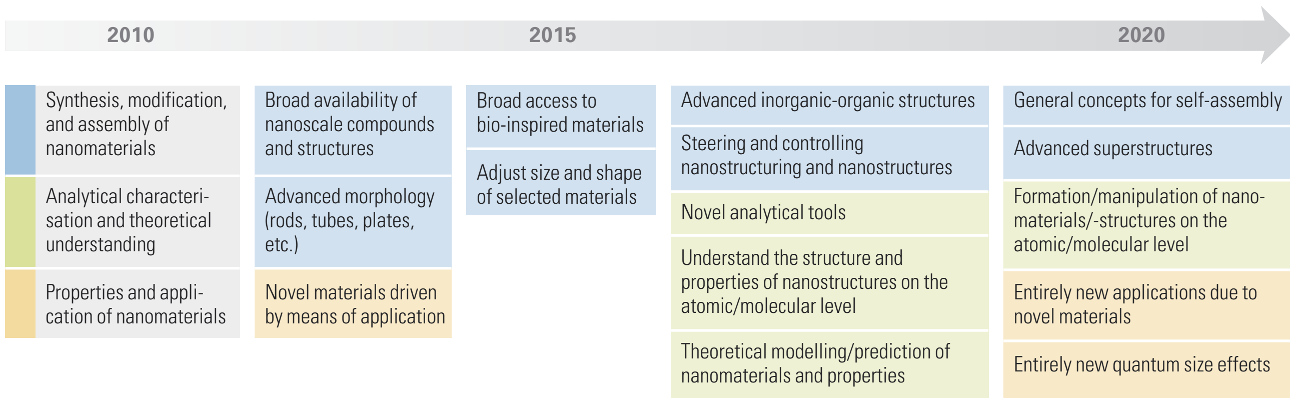

Fig. 3.7.4: Research roadmap.

c) Surface modification and conditioning

- Analyse local situation (e.g. bond strength, bond distance, coordination) on a (near) atomic scale;
- Analyse bonding situation at surfaces and of composites (e.g. coordination, adhesion, and adsorption);
- Correlate surface conditioning and properties of nanomaterials/ nanostructures.

d) New tools: high throughout experimentation and screening.

Conclusions and recommendations – European research programme

Concerning the potential development for new "inorganic – organic nanohybrid materials": "There's plenty of room in the middle"!

A future European research programme should address the following aspects:

- Choose and control type, concentration and location of defects and dopants; correlate type, concentration and location of defects and dopants with the properties of nanomaterials/-structures;
- Develop novel analytical tools and techniques;
- Realise tunable material properties depending on size and shape, preferably by external forces;
- Understand structure and properties of nanostructures on atomic/ molecular level; model and predict structures and properties theoretically;
- Self-assembly for advanced superstructures and biomimetric materials;
- Formation/manipulation of nanostructures on atomic/molecular level;
- Entirely new applications due to novel nanomaterials/-structures

3.8. COATING MATERIALS

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[Affiliations chapter 12]

As a cross-disciplinary field, surface technology is very important to all industrial sectors (see Fig. 3.8.1). The functions of coated substrates in greatest demand and where the biggest research input will be necessary in the next 10 years are:

- Easy-to-clean, self-cleaning, (anti-stain, anti-soil, anti-fingerprint);
- Sensor/actor properties, activity, switchability;
- Tribology;
- High temperature resistance;
- Hardness, elasticity;
- Corrosion/chemical resistance;
- Optical properties.

Coating deposition technologies provide enabling methods to manufacture nanostructured materials and coatings. Such systems offer the potential for significant enhancements to engineering and usage properties. These properties are the result of a reduction in micro-structural features within the coating or material by factors of 100 to 1000 times compared to current engineering materials and new material combinations.

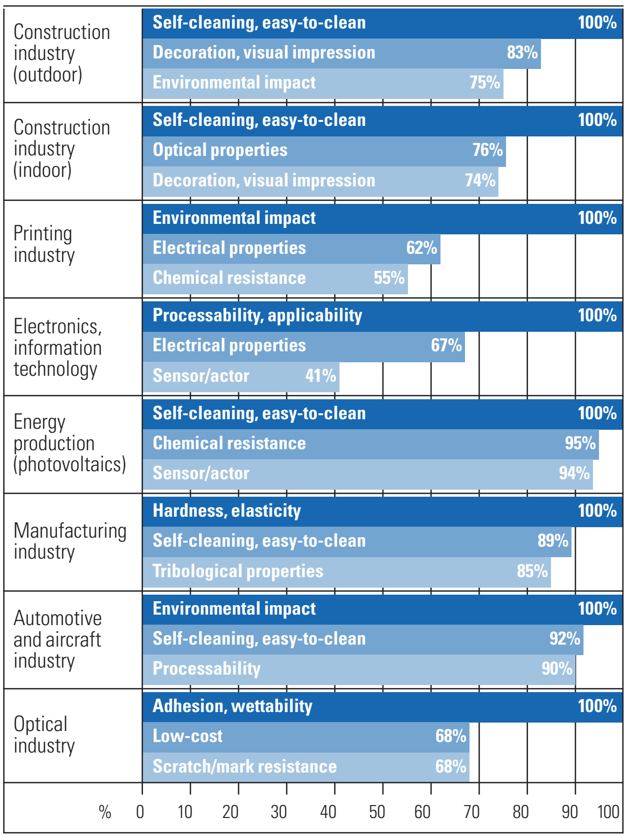

Fig. 3.8.1: Forecast of the demand of research in the field of coating materials (relativ prominence), broken down into eight industrial sectors.

The potential benefits include higher hardness and strength in metals, intermetallics and cermets resulting from reduced grain size and the ability of such nanostructures 'to tie up' dislocations, thus modifying material slip mechanisms (see Fig. 3.8.2). In nanostructured ceramics, higher hardness and toughness are accomplished with reduced defect size and enhanced grain boundary stress relaxation, even at room temperature. Diffusivity can be greatly increased, associated with a larger volume of grain boundaries. Thermal conductivity may be reduced due to enhanced phonon scattering from nanoscale features such as grain boundaries, atom clusters and other structural imperfections.

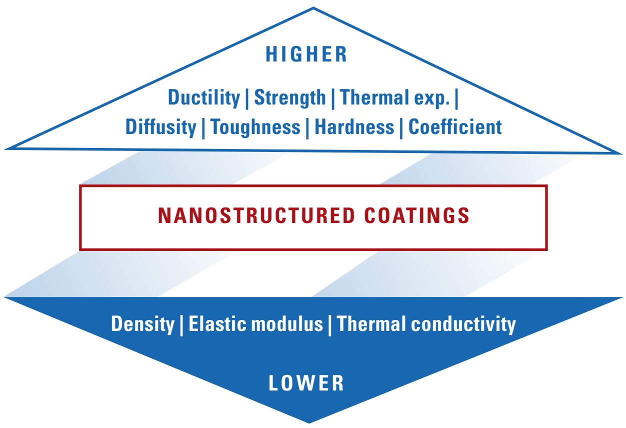

Fig. 3.8.2: Property enhancements as a result of nanostructured coatings.

Nanocoating technologies will permit the tailoring of coating performance to meet future engineering needs. These technologies will permit the incorporation of multiple material properties in a functionally gradient coating design, for example a self-diagnostic, thermal barrier coating system could be designed to have strain tolerance, low thermal conductivity and, through the incorporation of thermo-luminescent phosphors, will be able to measure metal temperature, ceramic surface temperature and heat flux.

3.8.1. POTENTIAL NANOSTRUCTURED COATING MATERIALS

Advanced thermal barrier coatings

Thermal Barrier Coatings (TBC's) are some of the most important 'nanostructured' coatings in service today in some of the most arduous service conditions. TBC's are used extensively in gas turbine applications to insulate superalloy turbine blades and vanes from the hot gas stream. There is a need for thermal barrier coatings with improved durability and performance (see Fig. 3.8.3). Current technology consists of layered structures, which incorporate a bond coat, designed to match the expansion of the ceramic topcoat to the base metal whilst providing the chemistry to grow a self-repairing alumina barrier layer onto which a strain-tolerant (if produced by EB-PVD) ceramic layer is deposited. The TBC is designed to resist heat flux and current designs result in temperature drops of 80–120°C across 200 m of ceramic. Future designs need to lower the thermal conductivity substantially (1°C/micron thickness should be a design aim), i.e. 200°C across 200 m of ceramic. The surface should retain its strain tolerance at temperatures up to 1500°C, resist sintering and be chemically resistant to CMAS attack (calcium magnesium aluminium silicate). None of these can be achieved at present.

Coating programmes	Critical nano-structured property	Component/ engine benefit
Co-WC wear-resistant coating	Increased hardness	5X life
Erosion/moisture-resistant coating for polymer matrix composites	Increased hardness Increased adherence	5X life Higher allowable
High temperature, crack-resistant coating	Increased strength Interface crack blunting Oxygen impermeable layer	3X life
Advanced thermal barrier coating	Reduced conductivity	+2% thrust/weight -1% fuel consumption

Fig. 3.8.3: Performance improvements for selected gas turbine applications of nanostructured coatings.

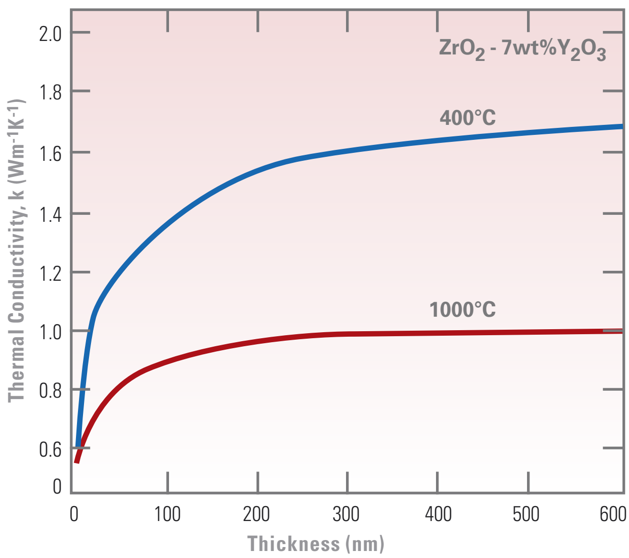

Fig. 3.8.4: Thermal conductivity of ZrO_2-7wt%Y_2O_3 TBCs as a function of coating thickness.

It should be possible to develop TBC's with improved performance, by reducing thermal conductivity using nanostructured ceramics. This results from the enhanced phonon scattering at nanodimension grain boundaries. Theoretical calculations indicate that nanostructured TBC's could result in thermal conductivities as low as 0.6 W m^{-1} K^{-1} (see Fig. 3.8.4). It should be further possible to strengthen the boundaries by refining the surface texture and structure at this nanoscale. Self-diagnostic nanothermal barrier coatings incorporate the benefits of a TBC, coupled with the ability to measure temperature, heat flux, phase change, ceramic loss or chemical attack. The incorporation of thermographic phosphors permits temperature to be measured at the TBC surface and also within the ceramic topcoat. An accuracy of 5°C can be achieved at up to 1000°C currently. This capability needs to be extended to 1500°C and would permit TBC surface and TBC interface temperatures to be measured in a running engine and thus the calculation of heat flux. Such on-line diagnostics would permit active cooling management in industrial power plant, improving efficiencies and therefore reducing emissions.

Nanostructured corrosion resistant coatings

- Many modern corrosion protection coating systems for automotive, aerospace and aero engine applications are engineered at the microscale. It is now common practice to first coat a component with a sacrificial layer (e.g. zinc on steel) before over-coating it with a multilayered, multi-component polymer coating (the paint system on a modern motor car works this way and is warranted for years). Future polymeric topcoats, should be designed to incorporate 'macro-molecules', polyacrylic acid that can selectively compete for metallic sites. This provides a self-repair capability to the polymer topcoat. Such binder molecules incorporated in the polymer topcoat compete for adsorption sites, improving adhesion and reducing environmental access.

- An alternative approach is to apply nanostructured physical vapour-deposited coatings as 'environmental barrier coatings'. Due to the cost of such treatments, it is normal practice to combine such barrier coatings with another functional need. A major application of such nanostructure PVD ceramic coatings addresses 'tribocorrosion' conditions, combining the requirements of erosion/wear resistance and an environmental barrier. Many nanostructured, super lattice coatings have been developed to combat 'tribocorrosion'. PVD and CVD ceramic-based coatings (e.g TiN, TiAIN, TiAICr NC etc) provide excellent environmental barriers, provided the coating remains intact. Coating adhesion, under aqueous service conditions, relates to inherent manufacturing defects, nearly always these coatings contain through-coating pores. Such pores allow direct access of the environment to the substrate, such that in time, corrosion protection is lost locally. Multi-layered, nanostructured coatings, as well as resisting wear, can be engineered such that re-nucleation during coating growth ensures that such through-coating defects rarely coincide. The incorporation of active metal inter-layers can also provide cathodic protection. This can be done by producing reaction products that limit environmental ingress.

- Smart high temperature corrosion resistant coatings work on similar corrosion inhibiting principles. The coating system is functionally gradient in design. The outer part is high temperature alloy optimised to grow a protective alumina scale. Under this is a region richer in chromium, which, when in contact with molten salts as a result of hot corrosion, responds to the chemical activity gradients generated in the melt and preferentially forms chromia scales, which minimise hot corrosion attack.

The above topics illustrate how, by understanding the mechanisms of degradation and chemical interactions at the atomic/molecular level, nanostructured and functionally gradient coatings can be designed to combat corrosion under aqueous, high temperature and/or tribo-corrosion conditions.

Low surface energy coatings

- Offer self-cleaning capabilities;
- Dominated by hydrophobic nanolayers or autocatalytic coatings at room temperature under atmospheric conditions;
- The former resists wetting by water, and dirt/grime is removed with the water droplets;
- Often termed the 'Lotus' effect, super-hydrophobic coating systems incorporate nanostructured surface relief (consisting essentially of structured pillars) over-coated with a hydrophobic material (waxy in its behaviour);
- Potential markets for these coatings include windows, automobile paints and glass.

Coatings incorporating optically active and/or electroactive nanoparticles

Provide various functionally enhanced properties:

- Incorporating ultraviolet adsorbing materials (e.g. ZnO and TiO_2) makes it feasible to design optically transparent coatings that do not transmit ultraviolet light;
- Such coatings can provide sun protection and be incorporated in smart window designs aimed at solar and solar/thermal energy management;
- Incorporating antimony tin oxide (ATO) into coating systems provides electromagnetic interference (EMI) or electrostatic discharge (ESD) protection;
- Additions of vanadium niobate can be tuned to provide switchable infra-red reflectivity.

In these latter aspects, much research is required into the identification of nanoparticle properties that can be actively incorporated into future coating systems.

3.8.2. COATINGS MANUFACTURING

Barriers to progress include:

- Materials availability;
- A commercially applicable process;
- Process reproducibility;
- Cost of materials and effectiveness of the manufacture.

The solution requires:

- Selection of the optimum deposition process (see Fig. 3.8.5);
- Choice of processing parameters for both compositional and microstructural control;
- Selection of materials and deposition parameters for interface engineering in multilayered structures;
- Optimisation of materials and deposition parameters to enhance structural stability at all operating temperatures.

Applications may include (see Fig. 3.8.6):

- Nanostructured, 'smart' corrosion resistant coatings that respond to the local chemical potential;
- Self-repairing paint systems; self-cleaning, anti-graffiti coatings;
- 'Smart' photochromic window systems.

It will be necessary to ensure successful transfer of these technologies from the laboratory (research base) out into industry and to demonstrate their technical and economic viability on a commercial scale.

Multi-functionality

Multi-functionality (e.g. easy-to-clean combined with scratch resistance or hardness and elasticity coupled with switchability) of coatings will be a key target of research in this field for the next decade. Meeting these demands requires the development of new and advanced materials and processes. The most important areas of research are:

MAGNETRON SPUTTERING
ELECTRON BEAM PHYSICAL VAPOUR DEPOSITION
CATHODIC ARC EVAPORATION
LASER ABLATION
CHEMICAL VAPOUR DEPOSITION
CHEMICAL SYNTHESIS
GAS PHASE SYNTHESIS
SOL-GEL
PLASMA SPRAYING
SOLUTION PRECURSOR SPRAY DEPOSITION
HVOF THERMAL SPRAYING
ELECTROPLATING
ELECTROLESS DEPOSITION

Fig. 3.8.5: Deposition methods for nanostructured coatings.

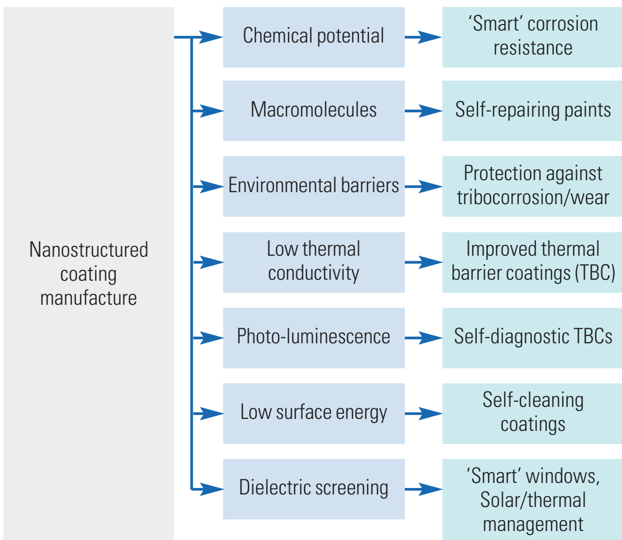

Fig. 3.8.6: Applications of nanostructured coatings.

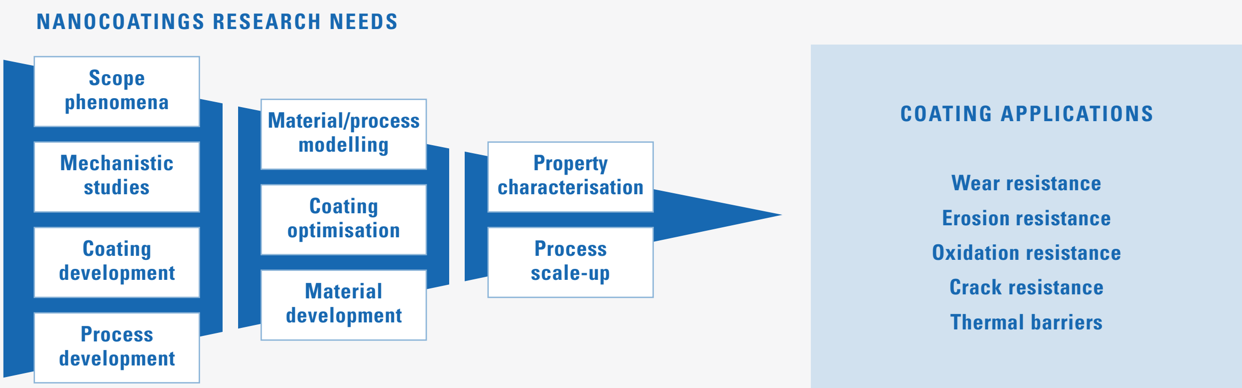

Fig. 3.8.7: Research targets to develop future nanostructured coatings.

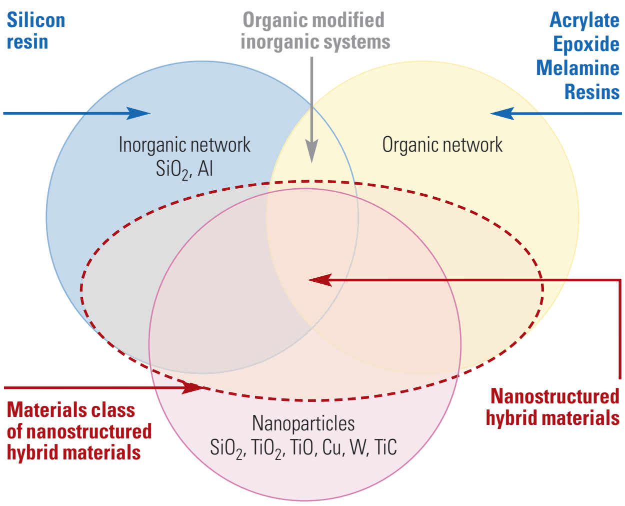

Fig. 3.8.8: Nanostructured hybrid materials.

- Hybrid materials with complex morphology (see Fig. 3.8.8);
- Nanocomposites, functional nanoparticles (e.g quantum dots, core-shell particles at different lengths scales, catalytic particles);
- Functional materials (inorganic, metals, alloys, polymers and DLC);
- Micro- and nanostructured materials and surfaces.

Nanocoating systems technology requirements

- Identification of suitable European technology bases;
- Identification of pilot applications – driven by a cost/benefit/risk analysis;
- Processing of engineering nanomaterials;
- Generation and evaluation of nanocomposite engineering properties;
- Demonstration of cost-effective manufacturing feasibility.

The main challenge of surface technology in the coming years will be controlling the increasing complexity of the coating materials and the associated coating processes. The necessity of developing new tools and methods to analyse these complex property profiles will demand significant development of advanced methods and simulation tools.

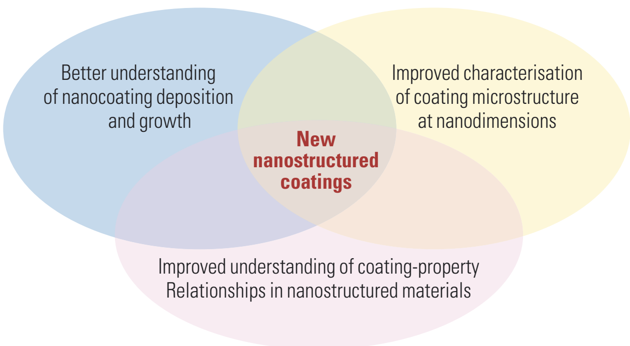

Fig. 3.8.9: Research needs for nanostructured coatings.

3.8.3. RESEARCH NEEDS FOR NANOSTRUCTURED COATINGS

Nanostructured coating materials and constituents will gain increasing importance as industrial coatings materials (see Fig. 3.8.7 and 3.8.9). Opportunities in the field of surface coatings research in the next few years will be:

- The investigation of structures at the nanoscale;
- The derivation of structure-property relations;
- The up-scaling to bigger lengths scales.

Organic and inorganic coatings containing nanoparticles will be further developed through:

- Advanced procedures combining vacuum techniques with non-vacuum coating techniques;
- New multifunctional coatings due to improved embedding of nanoparticles in the matrix and in-situ production;

- Increased study of particle-matrix interactions, particle distribution and self-assembly in thin organic and inorganic coatings (using surface sensitive techniques, like synchrotron radiation scattering).

The main problems to be solved before the adaptation of these nanocoatings to industrial processes are:
- Process costs;
- Reproducibility;
- Up-scaling to large substrate surfaces;
- Long-term stability of the coatings.

This requires new techniques in surface technology process control, using in-line analysis and process simulation at different length scales.

New research strategies exploiting synchrotron radiation and neutron sources

- Information on lateral and perpendicular dispersion or structure close to the surface;
- Contrast enhancement between components by anomalous scattering;
- Time-resolved in-situ studies of coatings under thermal and mechanical loads;
- Surface and interface sensitive neutron techniques using deuteration to determine chain conformations of polymer-coatings;
- Neutron imaging of conformation changes in the vicinity of nanoparticles;
- Combinatorial x-ray and neutron beamlines including optical spectroscopy and microscopy;
- X-ray nanobeam technologies for spatially resolved information.

To overcome the most challenging barriers in nanocoating materials and processing, a "GENNESYS Centre for Functional Coating Design" appears mandatory (see Fig. 3.8.10). This will require the establishment and substantiation of scientific drivers, robust application-driven research, and disciplined concurrent engineering through to prototype manufacture.

This technology centre should be led and supported by industry. As many fundamental problems have to solved, a very intimate interaction with the science centres "Functional interfaces" and "Precision synthesis" is most important. An appropriate and efficient platform for a regular exchange between these centres must be installed.

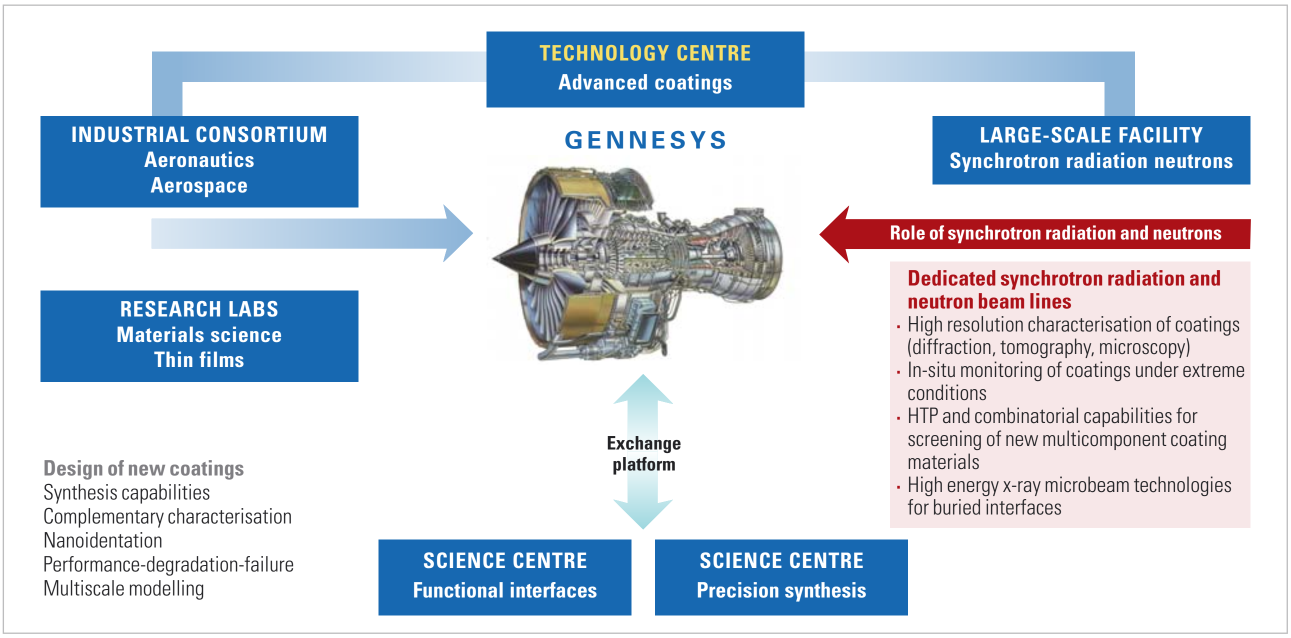

Fig. 3.8.10: GENNESYS centre for functional coating design.

3.9. DIRECTIONS FOR NANOMATERIALS RESEARCH

AUTHORS: H. Dosch, M.H. Van de Voorde
[Affiliations chapter 12]

For the welfare of society and economy in Europe, it is necessary that the prospective advanced nanotechnologies are realised; this will demand new and innovative nanomaterials and materials properties for a wide spectrum of applications. It is evident that the discovery of such nanomaterials will require fundamental research: "engineering structures at the nanoscale are far too complex for 'black art'" and the GENNESYS study shows that synchrotron radiation and neutron methods promise to be vital tools. The nanomaterials community is well aware of these needs and strongly wishes and promotes a close collaboration with large-scale facilities in the future. GENNESYS offers the opportunities for a friendly nanoscience – large-scale facility environment/platform and paves the ways for successful engagement.

Structural nanomaterials challenges

In Europe, we are blessed with some of the best facilities in the world but important adjustments are required to optimise them so as to make a major contribution in the field of nanostructural materials and to give Europe a competitive advantage.

As microstructure scales are reduced, new techniques are required to image and probe them. This requires significant efforts and requires working hand in hand with instrument scientists at synchrotron radiation and neutron facilities.

In particular, there is a need to:

- Develop research facilities which provide direct access to industry and research and development engineers and allow realistic processing and in-service conditions to be simulated;

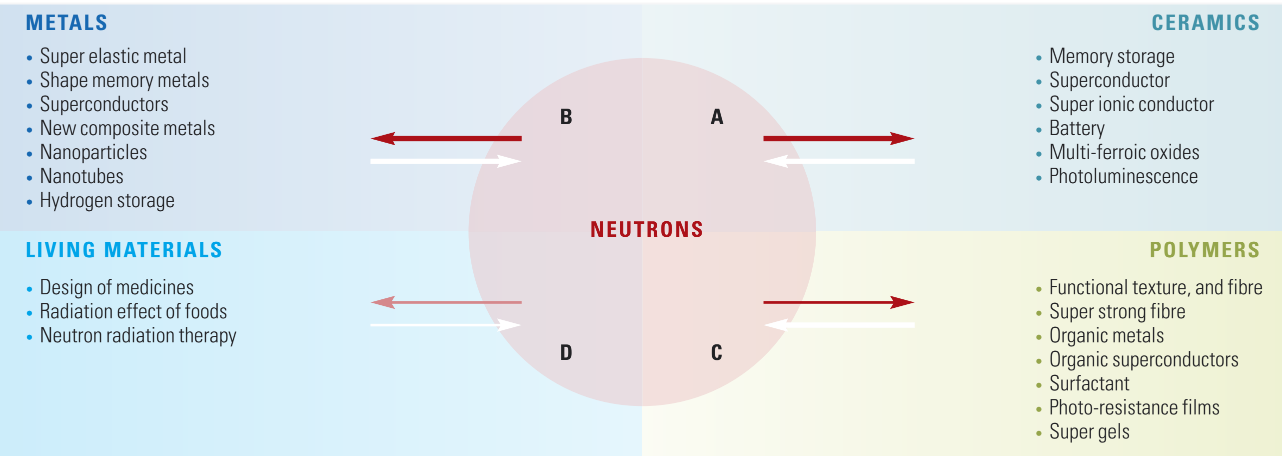

Fig. 3.9.1: Neutron science applied to "Nanomaterials science": metals, ceramics, polymers and soft materials for life science.

Important research areas for neutrons in nanomaterials science are summarised as follows:

- Nanostructural analysis of crystals, including the dynamical structure of magnetic and oxygen atoms, is indispensable for new materials development of high temperature superconductors, multiferroic devices, as well as magnetic memory devices.
- High resolution diffraction profile analysis becomes a standard method to characterise the residual stress measurement for metallic structural products.
- Complex molecular assemblies are characterised by small angle neutron scattering using the contrast variation technique combined by the selective H/D substitution.
- Inelastic neutron scattering to determine hydrogen motions in DNA is essential to solve the living function in order to design medicines.

This section focuses on the collaboration between mechanism philosophies and has worked out schemes for the three (nanometallic-, ceramic and polymeric) materials groups separately because of the difference in progress with nanomaterials and familiarity with large-scale facilities by the various scientific communities.

- Develop higher-resolution beams: down to submicron sizes for synchrotron radiation and down to 100 microns or better for neutrons, for the study of fine-scale structures, thin films and coatings;
- Assure the capability to manipulate and process materials at the nanoscale in-situ at synchrotron radiation and neutron sources;
- Develop in-situ environmental and temperature control for performing experiments, allowing real-time simulation and monitoring of material fabrication, industrial processing and nanostructure development;
- Build synchrotron radiation and neutron instruments capable of studying not just samples but devices and components operating under realistic conditions;
- Build dedicated beamlines with sufficient physical space to house prototype process plants, large engineering samples and sample manipulation devices;
- Assure faster experiment turnaround at facilities in order to accelerate product development with industrial and academic involvement;
- Establish greater collaboration between facilities, academics and industrial teams in designing/carrying out experiments - this would be aided by a pioneering GENNESYS Structural Nanomaterials

Centre providing leadership and unique nanomaterials processing and handling facilities;
- Develop improved software tools for experimental planning, design, implementation and data analysis, so that a greater proportion of beam time can be used to obtain useful data;
- Create better links between: basic research, materials characterisation, materials engineers and end users;
- Improve the interface between international research facilities and the industrial and engineering community. Such facilities have traditionally been focused on the delivery of fundamental science with little liaison to industry.

Much of the nanomaterials research which will be of benefit to industry is non-proprietary and can be disseminated to the benefit of the wider industrial science community.

Functional nanomaterials challenge

Impacts in the short- and medium term (coming 10 years): "the step from scientific research to technological application". Hence we deal with "industrial" issues and projects:
- High-k dielectrics to push conventional CMOS scaling 1–2 generations further;
- Parasitic resistances and parasitic capacitances in densely packed devices;
- Magnetic recording and storage: New concepts such as domain wall control to increase memory density. Non-volatile memories with low power consumption and without moving parts, especially for mobile operation;
- Photonics to switch from electrical to optical data transfer for short and medium distances: development of materials and devices (emitters, modulator, detectors).

For all these developments, functional nanomaterials are at the very core, and characterisation and control of fabrication are key issues. Synchrotron radiation and neutron scattering are extremely important tools in this process. Key techniques that need to be developed to a high standard and made available for "routine" use are:
- X-ray nanobeams with diameters of 10 nm or below to combine high spatial resolution with the high resolution on momentum transfer (Fourier space), which is the main strength of scattering techniques;
- Coherent scattering for full 3-D reconstruction of real space sample structure without simplifying model assumptions, ultimately with atomic resolution;
- Combination of scattering, imaging, and spectroscopy on the same sample spot for considerable gain of sensitivity;
- Magnetically sensitive scattering techniques with small beams for selective investigation of nanostructured magnetic materials;
- Time-resolved studies to follow dynamic processes like domain wall propagation, diffusion, spin precession, surface formation/transformation, chemical reactions etc. in real-time. The use of intense pulsed beams is crucial here, and free electron lasers will certainly push this field;
- X-ray excited optical luminescence from single nanostructures;
- Intense neutron sources:
  - Upgrade of continuous wave (cw) sources;
  - Powerful European spallation source;
- Highly controlled manipulation of single nanostructures;
- In-situ processing and characterisation.

The longer term views (up to 20 years): Basic science oriented research. Although we aim to make a forecast, one has to be prepared to react flexibly to new developments:
- Develop alternatives to the Si mainstream technology. Concepts like molecular electronics or the use of carbon nanotubes or graphene for transistors might still seem utopist;
- Combination of Si with other materials, where they have superior properties, like III-V-compounds for optoelectronic applications. A very promising route seems to be the fabrication of nanowires, which circumvent many problems of epitaxial growth by a small contact area to the substrate;
- High temperature superconductors: recently several promising materials have been developed, and substantial progress is foreseen by a combination of these materials in layers. This might lead to a similar development as for semiconductors in the last two decades, where the combination of different materials in thin layers has allowed tailoring of material properties that cannot be reached with one material alone;
- Exploiting not only the charge of electrons for device operation, but in addition their spin, allows to build completely new devices, which might revolutionise the way computers are built or data are transmitted.

Nanopolymers, biopolymers and bionanosystems challenges

Elements for which synchrotron radiation and neutrons will lead to future breakthroughs of nanopolymers, biopolymers and bionanosystems:
- Wavelength ranges of radiation ideally matched to allow atomic to molecular length scales to be probed;
- Energy of radiation allowing atomic and molecular dynamics to be studied;
- Current new generations of synchrotrons provides flux and hence measurement rates where real-time kinetics and dynamics can be probed;
- Bright sources to allow measurements of microscale samples;
- Radiation can be non-invasive (particularly true for neutrons), allowing many in-situ and in-vitro (and possibly in-vivo) measurements to be followed;
- Variety of measurement conditions at the sample are possible – temperature, pressure, pH, external fields (electric, magnetic, shear, etc) concentration.

Future beam line developments i.e. bio-nanomaterials

(see Fig. 3.9.2)
- Combined in-situ analysis;
- Development of grazing incidence scattering;
- Polarisation analysis (incoherent scattering removal);

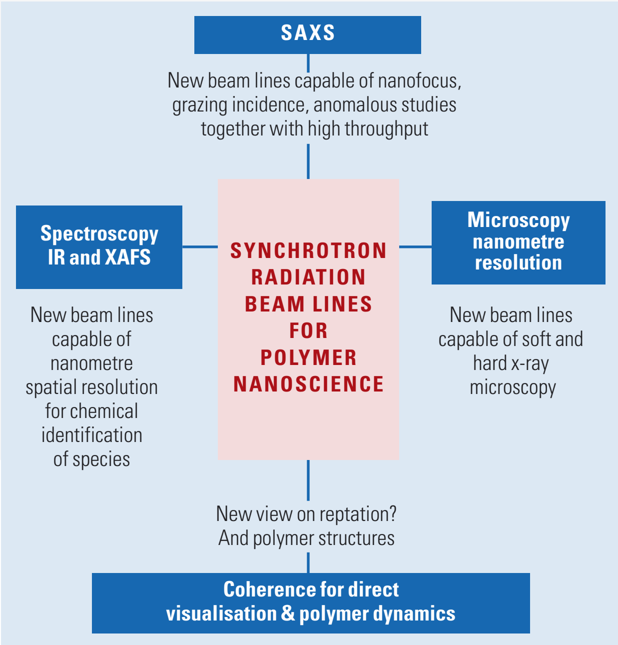

Fig. 3.9.2: Beam line spectrum for bio-nanomaterials research.

- Surface quasi-elastic scattering instruments;
- Routine ultra-small angle scattering capabilities.

- **Experimental developments**

The new nanomaterials science and technology demands new developments in detection, optics, computing, and sources. This is schematically represented in Fig. 3.9.3.

Conclusion

Know-how in nanotechnology will be a key factor determining the international position in economical, ecological and social terms. Synchrotron radiation and neutron centres are essential in this process: they provide major research capabilities, and provide a stimulating environment, ideal to host GENNESYS nanomaterials technology centres, where scientists and engineers perform cutting-edge research and develop tools and methods to be used in science and industry laboratories.

Supporting the individual research efforts that will underpin progress in the understanding and implementation of nanomaterials will require steep changes in the capabilities of current synchrotron radiation and neutron sources, and rapid evolution in the ways in which

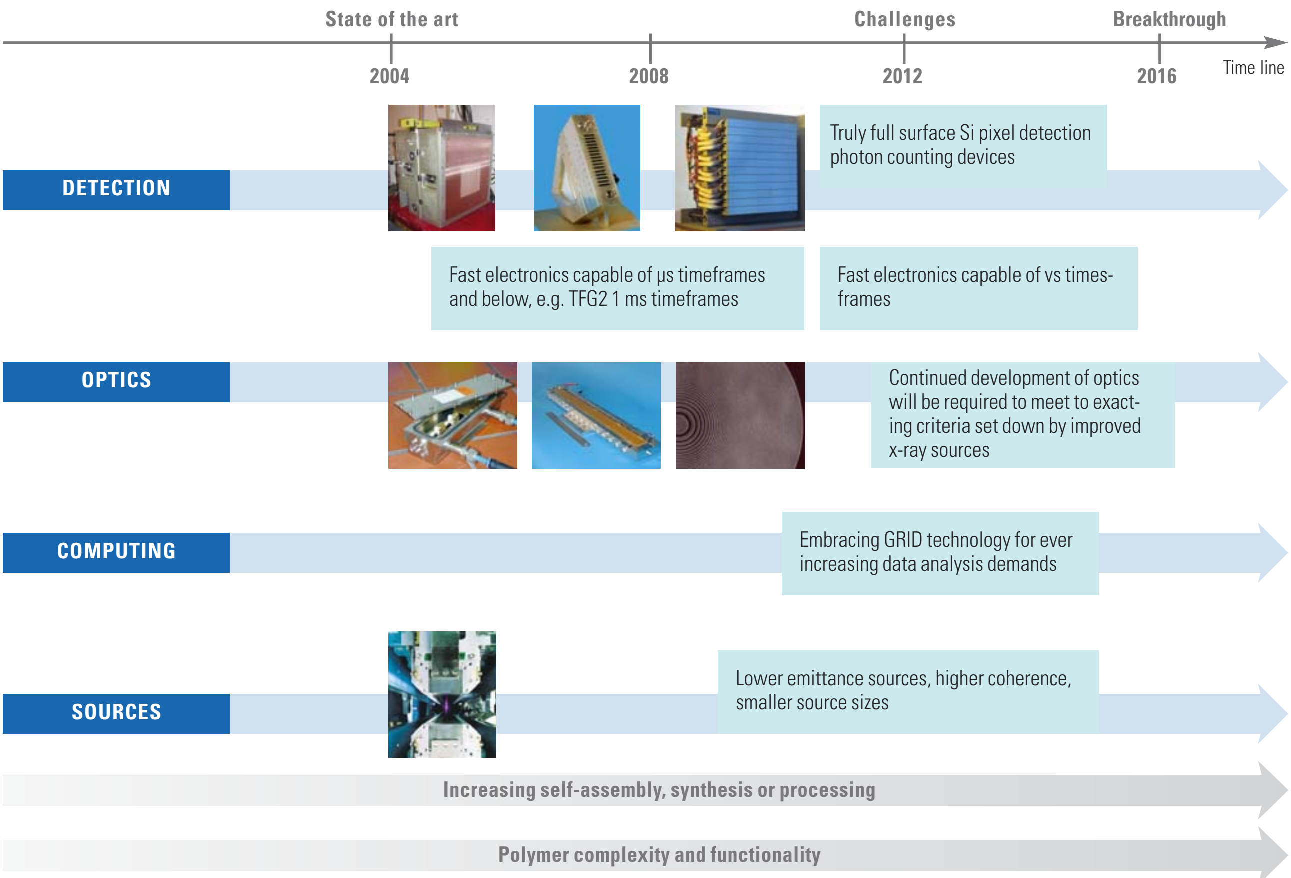

Fig. 3.9.3: Schematic representation of the new nanomaterials sciene and technology demands for new developments in detection, optics, computing and sources.

these facilities interact with industry. There are exciting challenges to be addressed to the benefit of the international facilities, academic partners, industrial end-users, and the wider European Economic Community. The GENNESYS study has provided an overview.

European Research Initiative

In order to implement the scientific and technological outcomes of the GENNESYS study, a European research initiative is required, with the following important elements (see Fig. 3.9.4):

Basic nanoscience needs

- Upgrade of third generation synchrotrons:
  - High-brilliance beamlines with nm-diameter x-ray beams;
  - Combination with scanning probe microscopes directly in the beam;
  - In-situ preparation and in-situ growth.
- Beam lines devoted to nanoscience and nanotechnology;
- GENNESYS nanotechnology centres at synchrotrons;
- Free electron lasers and synchrotron sources for time-resolved studies:
  - Track processes on picoseconds to hours timescale;
  - Use of coherent beams.
- Upgrade continuous wave (cw) neutron sources:
  - Polarised neutron scattering.

Fig. 3.9.4: European initiative for a nanomaterials – large-scale facility research platform.

- European spallation source:
  - Work with smaller sample volumes.
- Trained scientists and engineers;
- Close collaboration with scientific labs.

Applied research and industrial development needs

- **Education and exploitation**
  - Train scientists from PhD level in the use and methods of nanofunctional material science and, in particular, synchrotron radiation and neutron facilities;
  - Create awareness of capabilities also at the engineer and management level;
  - Transfer knowledge to companies through educated scientists and engineers;
  - European institutes to coordinate research efforts.

- **Impact and benefits for Europe**
  - New materials for energy production and more efficient energy use;
  - Minimising environmental impact due to improved fabrication methods ("green technology"), improved monitoring systems;
  - Improvements in health care and medical diagnostics;
  - Security and surveillance systems;
  - Keep European research and technology competitive.

At present, the situation in Europe for exploiting synchrotron radiation and neutron sources for nanomaterials research is disjointed. It is not certain that Europe will be an international leader in the field in 10 year's time. There are significant threats to the development of a cross-European research programme to build upon existing expertise and success. The current position can be optimised as shown by the SWOT chart in Fig. 3.9.5.

Without a concentrated European initiative, it is unlikely that nanomaterials will have sufficient critical mass and momentum to deliver radical new design concepts and step jumps in performance. One way forward is to bring together, in a European initiative, engineers and instrument scientists across both neutron and synchrotron platforms to create an integrated GENNESYS Centre for Structural Nanomaterials and an important research programme.

STRENGTHS
- World leading facilities
- High level of expertise
- Strong engineering focus at some facilities
- Large user base

WEAKNESSES
- Few beamlines dedicated to engineering studies
- Not proactive in engaging with industry
- Scientific outputs valued over engineering promise

OPPORTUNITIES
- New facilities coming on-line
- Neutron & synchrotron x-ray methods have potential to provide unique insights
- Global market for nanomaterials increasing

THREATS
- Japan and US will overtake Europe
- Instrument development too slow for nanomaterials
- Poor communication between instrument scientists and engineers

Fig. 3.9.5: SWOT chart for Europe's current position in nanomaterials research.

4. SPECIFIC CHALLENGES FOR NANOMATERIALS ENGINEERING

4.1. OVERVIEW

AUTHORS: H. Dosch, M.H. Van de Voorde
[Affiliations chapter 12]

Nanomaterials science and technology has so far focused activities on the synthesis/processing and nanoparticles/materials characterisation with minimum attention to the nanoengineering aspects; the latter are tackled mainly by trial and error procedures. Nanoengineering activities are based on the development of new knowledge (nanoscience), new "made" things (nanotechnology) and new ways of working (nanopractice), schematically represented in Fig. 4.1.1.

In addition, the mechanical testing of nanomaterials and components is limited to ideal laboratory conditions; exposures to simulated industrial environments have not been done due to the lack of test equipment and complex test procedures.

This chapter gives an overview on nanomechanical engineering and design and provides some insight in the:

i) Optimum design with nanomaterials;
ii) Study of their mechanical and oxidation/corrosion properties;
iii) Engineering properties such as nanotribology and nanojoining;
iii) Behaviour of nanomaterials and components in in service operating conditions.

In materials engineering research, synchrotron radiation and neutrons could play an important role in the future, in particular on challenging time- and lengthscales, in the understanding of the fundamental mechanisms of creep-, fatigue-, crack initiation/growth and fracture modes. This chapter highlights the research needs for reliable design and safe process operations and finally to engineering progress i.e. in studies of reliability, plant performance, life time prediction, failure analysis, leading up to industrial innovations. It is of great importance that steps are undertaken to realise an advanced modern infrastructure for nanomaterials engineering studies at large-scale facilities.

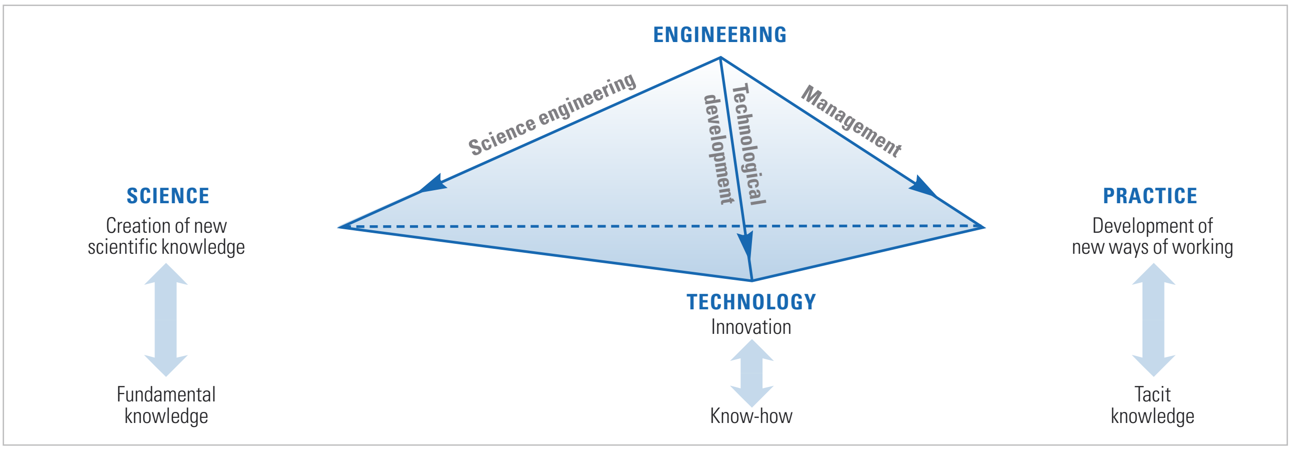

Fig. 4.1.1: The essence of nanomaterials engineering.

Fig. 4.1.2: Overview: bridging nanoengineering between basic sciences and the industrial nanotechnologies.

4.2. MECHANICAL ENGINEERING AND DESIGN

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The unique properties of nanoscale metals offer significant prospects for new applications as advanced structural materials. The novel properties and associated functionalities arising from nanoscale materials can only be fully exploited when a complete understanding has been gained by analytical investigation and characterisation. The knowledge of reliability and performance will provide a basis for developments of nanotechnological applications. Three important scientific/engineering areas, for which mechanical properties at the nanoscale play a significant role, have been identified (see Fig. 4.2.1 and 4.2.2):

Bulk materials with nanoscale microstructure or with nanostructured functionalised surfaces:
- Nanocomposite aluminium alloys for high-end transportation systems);
- Nanoporous metals for tailoring foams (high strength by decreasing the length scale);
- Nanocomposite coatings or coatings with extreme high fatigue;
- Nanostructured surfaces for bulk materials with self-adapting frictional properties.

Mechanical functional units on the nanoscale (Nano Electro Mechanical Systems, NEMS):
- Ultra-high sensitivity sensors;
- Nanoscale motors;
- Nanobiological devices.

These functional units experience more extreme conditions, such as high mechanical stress, high electric current densities, than their bulk counterparts. With decreasing size and mass, the resonance frequency of nanoscale mechanical devices increases, opening perspectives for frequencies up to the THz regime as well as challenges from new materials reliability and performance issues.

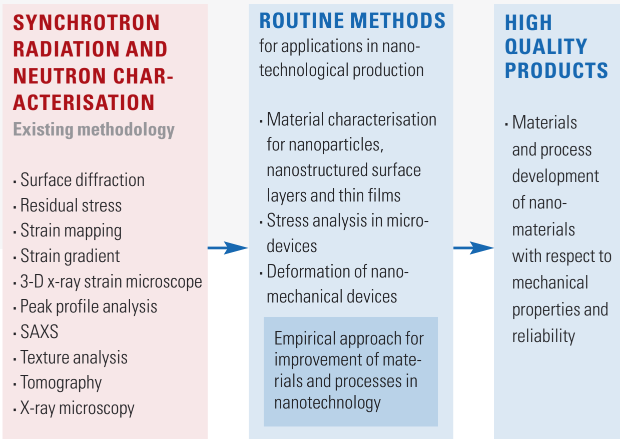

Fig. 4.2.2: Product improvement through characterisation of nanomechanical properties with synchrotron radiation and neutron methods.

In contrast to a single nanomechanical component, e.g. an individual nanotube, a functional nanomechanical system incorporates several components which need to be assembled in a well-defined manner. For this, however, a deep understanding of relevant processing procedures and interactive mechanisms is required.

Hierarchical structures down to the nanoscale:
Prominent examples are bones which have extraordinary mechanical properties combining high stiffness and strength with good fracture toughness. By learning from nature, the subtle structural elements have to be unravelled in order to optimise the performance of mechanical components.

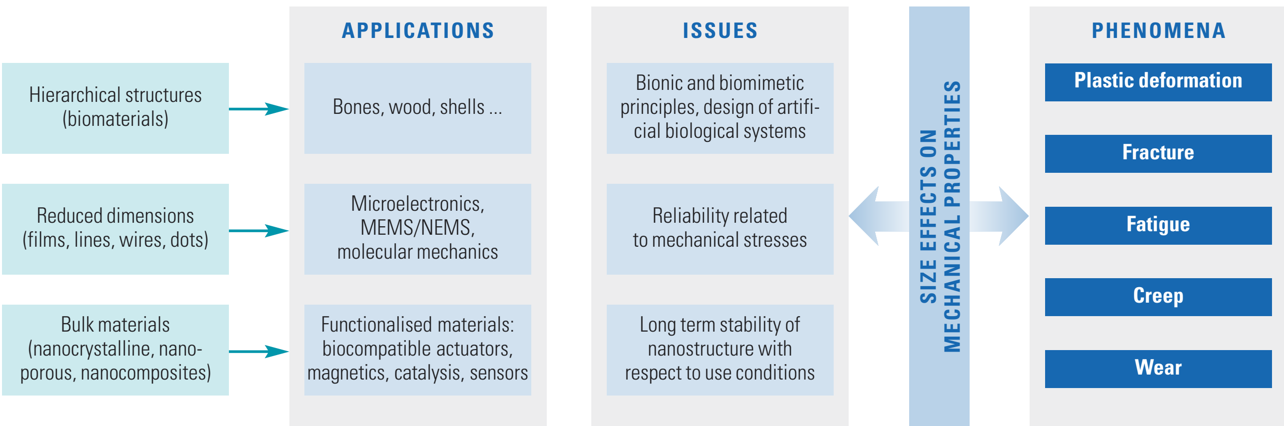

Fig. 4.2.1: Relation between engineering phenomena and the fundamental issues and applications of nanomaterials.

Knowledge base for nanomechanics

The fabrication and the manufacturing of advanced nanomaterials and nanostructures build the foundation of nanotechnology. The main challenge in manufacturing nanomaterials and nanostructures consists in aiming for a new access towards system design and manufacturing, taking into account the specific properties of nanomaterials and the new physical concepts in nanoscale technology. This requires (see Fig. 4.2.3):

- Systematic studies of mechanical integrity and joining of nanomaterials are of utmost importance for technologies;
- A comprehensive and interdisciplinary approach including a wide range of techniques and methods for characterisation;
- In-situ studies of nanoscale materials and systems for understanding the microscopic processes during operation.
- Development of stable and highly protective nanostructured coatings for applications with high temperatures by in-situ microstructural characterisation;
- Characterisation of nanoscale mechanical contacts with respect to adhesion, friction and wear in technical systems, and resulting in changes in material properties;
- Development of joining methods for nanoscale components and nanostructured materials by characterising joints with high spatial resolution;
- Study of nanofluidics and mechanics by measuring short-range ordering at solid-liquid interfaces including wetting and de-wetting processes;
- Role of the nanostructure of surfaces for the development of corrosion resistant coatings.

The ultimate goal is to design and to control fabrication based on the arrangement of individual atoms and molecules. The characterisation of the relationship between chemical composition, nanostructure, and resulting mechanical or functional properties is crucial in order to achieve materials with better or even completely new properties, and cost-effective systems with novel functionalities. It is necessary that the nanostructures have long-term stability in each different environment and with respect to the experimental and/or industrial conditions. To satisfy these needs, several key scientific areas can be identified, which will have a particular impact on the progress in a number of research topics:

- Development of "design rules" for the synthesis of nanostructured, possibly hierarchical materials, functionalised surfaces and nanomechanical devices;
- Artificial patterning of components and integration, or self-assembly of molecular mechanical components into nanosystems;
- Mechanical behaviour on the nanoscale with respect to the role of molecular interactions and defects in confined dimensions for the elastic, visco-elastic, plastic and fracture behaviour of nanostructured bulk materials, surfaces and nanocomponents;

4.2.1. MECHANICAL INTEGRITY OF NANOSCALE MATERIALS

(see Fig. 4.2.4)

Fatigue and fracture

Despite many years of study on bulk materials, the fundamental mechanisms of fatigue crack initiation and growth are still relatively unclear, mainly due to the lack of analytical techniques which provide the relevant spatial resolution. Here, new generation synchrotron sources and new revolutionary x-ray optics will offer the possibility of non-destructive studies at the nanoscale.

Deformation and creep

The grain size of new high-strength nanocrystalline materials is less than 100 nanometres. The creep behaviour of such nanocrystalline materials, however, is largely unclear. In order to better understand the mechanisms involved in determining the creep behaviour and, more generally, the mechanical response of nanocrystalline materials, the active deformation mechanisms have to be determined as a function of temperature and strain rate by in-situ studies.

EXPERIMENTAL DEVELOPMENT

Residual stress, strain mapping, strain gradient, 3-D x-ray strain microscope, peak profile analysis, SAXS, texture analysis, tomography, 3-D x-ray microscopy

In-situ studies for various loading conditions:

- Mechanical stress and pressure
- High and very low temperature
- Sliding contacts
- Cyclic loading
- Electric and magnetic fields for coupled electromechanical effects

Understanding of fracture and deformation as well as degradation of nanomaterials due to fatigue, creep and wear with special emphasis on microstructural instabilities

High resolution in space:

- Steep stress gradients at functional surfaces of engineering materials
- Stress distribution in nanostructured materials
- Strain mapping in nanodevices
- Degradation processes at flaws and defects
- Ultrathin films
- 3-D reconstruction of complete microstructure on nanoscale (3-D XRD)

Detailed understanding of relationship between structure, defects, microstructural instabilities and mechanical behaviour

KNOWLEDGE BASE

Materials and processes development of nanomaterials with respect to mechanical properties and reliability

Fig. 4.2.3: Creation of a knowledge base for the exploitation of nanomechanics.

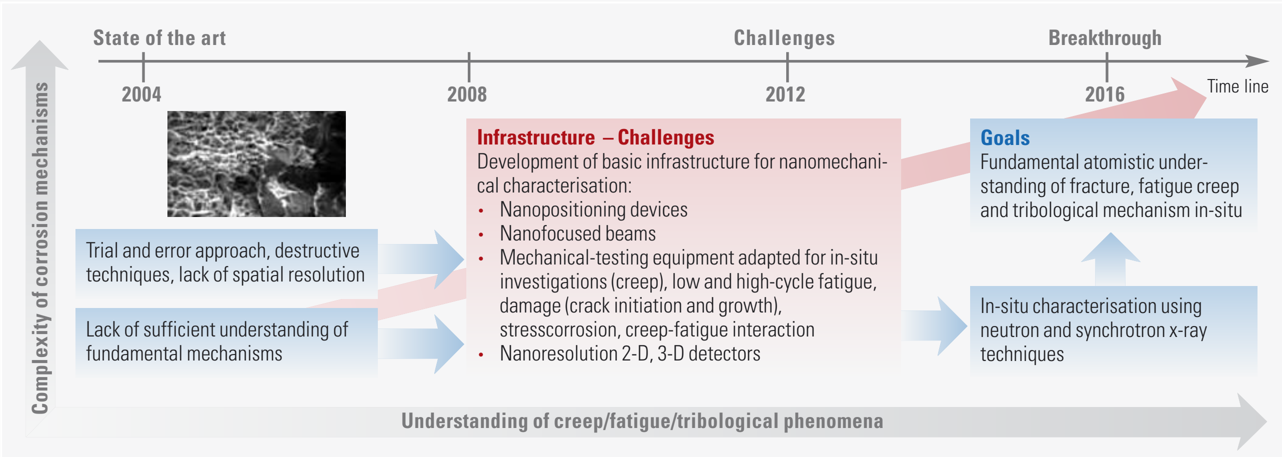

Fig. 4.2.4: The requirements for the understanding of fundamental mechanisms of fatigue/creep/terminological phenomena in nanomaterials.

Tribology and wear

It is obvious, that a fundamental understanding of tribology demands highly accurate materials testing capabilities for the very surface of the sliding components. In metallic materials, it has been shown that nanocrystalline surface layers are formed which determine the wear properties of the material. A fundamental understanding of the processes behind this observation will allow for designing nanostructured surfaces with tailored tribological properties.

4.2.2. JOINING OF NANOMATERIALS

In future nanotechnologies, the reliable joining of nanosized components in MEMS/NEMS applications and of materials with a nanocrystalline grain size in large scale components will play a key role. The established joining techniques cannot be extrapolated to nanomaterials, because the nanosize and the large surface/volume area alter their properties (melting temperature, surface diffusion) significantly. These nano- and microscale phenomena strongly affect the mechanical and physical properties of substance-to-substance joints.

It is crucial that the joining process does not alter the dimensions and/or properties of the materials. Therefore, the key challenges are to obtain in-situ information on structure and composition changes during processing and to monitor the temporal development of strain and microstructure. In order to be able to develop the joining of nanomaterials into a useful technology, the influence of heat and/or deformation on the nanostructure changes on short and very short time scales need to be clarified. Established joining processes need to be adjusted and novel joining processes need to be developed.

Future role of neutrons and synchrotron radiation facilities

Substantial basic research is needed to establish an engineering science base in nanomechanics. The instruments and techniques presently used for experimental micro- and nanomechanics are depicted in Fig. 4.2.5. and 4.2.6.

Conventional characterisation techniques are based on various types of scanning probe microscopy such as atomic force microscopy (AFM) and, especially for polymers and biological materials, laser scanning confocal microscopy (LSCM). Integration of force measurements and imaging capabilities in AFM systems and hybrid AFM-nanoindentation devices has been successfully applied for studying nanomechanics and technologically important material systems, including those used in magnetic storage, microelectronic and telecommunication devices, but are limited to surfaces and limited sample environment conditions.

Synchrotron radiation and neutrons are unique in allowing a non-destructive analysis of the phases, the microstructure and strain development during the joining process. In-situ studies during joining processes will allow to follow the evolution of the nanostructure and its eventual degradation during the joining process. Subsequent in-situ tests of the joints using synchrotron radiation under loading will provide information about the correlation between the nanostructure with physical and mechanical properties of the joints, leading to:

- Better understanding of bonding on the atomic scale;
- In-situ control of bonding and welding process;
- Microscopic understanding of failure;
- Develop of new solder material with a better match of thermal expansion coefficients.

Scattering experiments with synchrotron radiation or neutrons greatly complement the capability to the conventional microscopy probes:

- For complex nanomaterials systems, combinations of various scattering techniques are used to investigate the microstructure/morphology at various length scales, ranging from 1 to 100 nm. Such combined measurements enable hierarchical and highly anisotropic microstructures in materials – in fibre or clay-impregnated nanocomposites – to be fully characterised.

- Neutron and synchrotron x-ray diffraction are capable to measure the depth profiles of residual stresses with increasingly better spatial resolution. Residual stresses affect such important materials design properties as yield and fracture strength, microcracking and fatigue life.

- Diffraction methods are widely accepted as the most general and reliable non-destructive method of quantifying the residual stress tensor. They are based on the measurement of the distance of atomic planes of the crystalline grains within the material as very sensitive strain sensors. Detailed analyses permit separation of long-range macro-stresses and short range or grain-to-grain micro-stresses.

The envisioned support of nanoengineering and design by synchrotron radiation and neutrons is mainly based on diffraction measurements. Future developments will depend greatly on overcoming current infrastructural barriers:

- Improvement of beam stability and quality and the reduction of spot size by new x-ray optics combined with improved detectors (larger areas, smaller pixels, faster readout) would enable many of the proposed studies mentioned above for different applications and loading conditions, e.g. mechanical strain, pressure, temperature, corrosion environments.

- Dedicated beam lines with permanently installed and/or easily to altered standard mechanical testing equipment (i.e. tensile testing, tribometer, heat and cooling stages). Increase user-friendliness and availability, provide support infrastructure for sample preparation and complementary studies, and allow for long-term use and systematic studies.

- Higher resolution in space is needed for research on steep stress gradients at functional surfaces or at joints, for stress distribution in nanostructured materials and for strain mapping in NEMS.

- The development of synergistic tools between experiment, theory and modelling for improving analysis and interpretation in terms of microstructure and/or properties would result in a comprehensive understanding of microstructural instability.

- Dissimilar welds of nanomaterials provide a special challenge due to complex processes of phase formation and strains. Here, synchrotron radiation and neutrons are ideal probes for studying phase evolution and strain evolution, as well as optimising fillers and processes.

- Failure mechanisms in welded nanomaterials have, so far not been studied in detail. Synchrotron radiation tomography and diffraction will play a vital role in the determination of the failure mechanism and failure progress in welded structures.

- Nanomaterials present new challenges for joining technologies, since their properties can be changed drastically by thermal loading. Thus, new joining technologies need to be developed. Synchrotron radiation and neutrons can play a key role in these developments by revealing microstructure changes during non-destructive joining processes which take into account both spatial and time resolution.

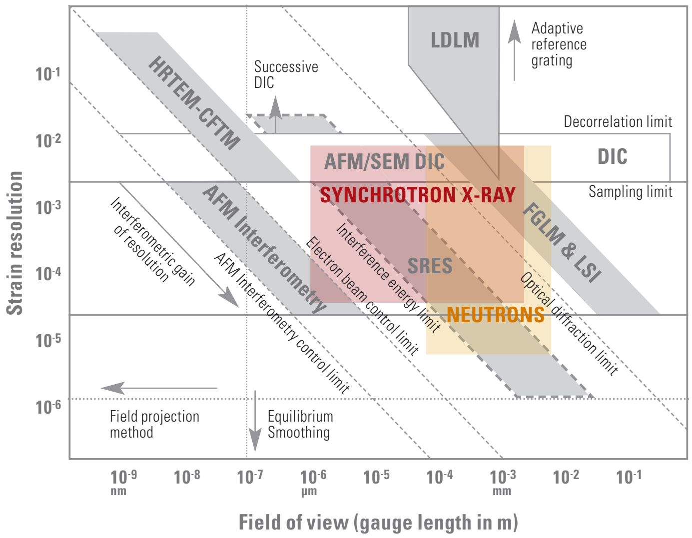

Fig. 4.2.5: Instruments and techniques for experimental micro- and nanomechanics HRTEM: High Resolution Transmission Electron Microscopy, SRES: Surface Roughness Evolution Spectroscopy, CFTM: Computational Fourier Transform Moiré, FGLM: Fine Grating Laser Moiré, AFM: Atomic Force Microscopy, LSI: Laser Speckle Interferometry, SEM: Scanning Electron Microscopy, DIC: Digital Image Correlation, LDLM: Large Deformation Laser Moiré

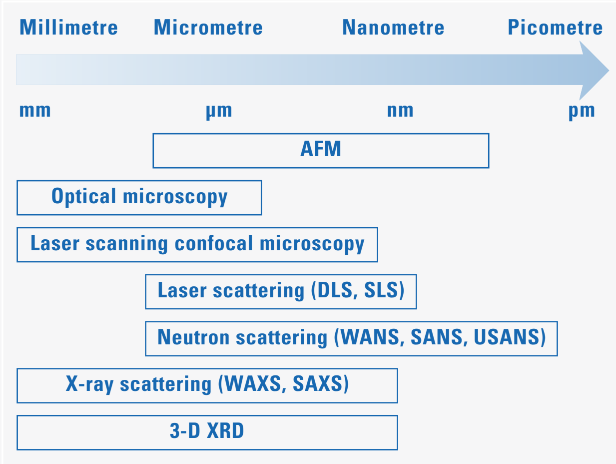

Fig. 4.2.6: Complementary analytical techniques for the analysis of nanomaterial integrity.

4.3. CORROSION AND PROTECTION OF NANOMATERIALS

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[Affiliation chapter 12]

The corrosion of nanomaterials (surfaces, interfaces, nanoparticles) is a basic chemical degradation process which takes place either in the earth's humid and oxygen containing atmosphere or in man-made technological processes.

Aqueous and high temperature gas corrosion of metal alloys used in construction work or in the car industry destroy more than three percent of the world's annual Gross Domestic Product. In addition, magnetic nanoparticles, employed in magnetic storage media, are affected in their magnetic properties by corrosion processes. On the other hand, through controlled electrochemical decomposition of metal alloys nanoporous materials with diverse technological potential can be produced, ranging from new catalyst materials to sensors. Finally, via controlled oxidation, ultrathin oxide films can be prepared, which serve as electron tunnel barriers in nanoelectronics. For the future, nanomaterials with a longer life-time and chosen corrosion/oxidation rate will be needed, as well as thermal and oxidation-protective, self-repairing coatings with increased performance controlled on an atomic level.

Therefore, tailoring and controlling nanomaterial corrosion, as well as the examination of deterioration mechanisms, plays a dominant role for key technologies such as corrosion protection, catalysis, gas sensing and large area surface nanopatterning. The different applications have in common that they imply processing conditions involving water or varying corrosive gas pressures ranging up the bar regime with temperatures up to 1500 K or higher, like in gas or aircraft turbine applications. Future development in the field of corrosion mechanism and protection of nanomaterials includes the following targets (see Fig. 4.3.1):

Targets:
- To develop new materials with improved corrosion protection for industrial applications;
- To understand the oxidation and corrosion processes on the atomic scale and on variable timescales;
- To develop corrosion maps for nano-"model" alloy materials under lab conditions;
- To make use of controlled oxidation/corrosion processes for large-scale surface nanopatterning for future bottom-up technologies.

Today's and future synchrotron radiation and neutron facilities provide a portfolio of different techniques which can deliver the desired information in-situ, in real-time, without destruction of the sample, as summarised in Figure 4.3.1.
- To predict the corrosion behaviour of nanostructured materials in service conditions;
- To improve the extrapolation from laboratory conditions to industrial processes.

In order to combine research and development in the field of nanomaterial corrosion and protection with synchrotron radiation and neutron based techniques, the following recommendations are given.

Recommendations for synchrotron radiation and neutron facilities (see Fig. 4.3.2)
- The creation of a science centre combining in-situ corrosion studies by synchrotron radiation and neutrons based techniques with state of the art theoretical calculations (Fig. 4.3.3).
- To implement in-situ corrosion sample environments at synchrotron radiation and neutron facilities, which combine synchrotron

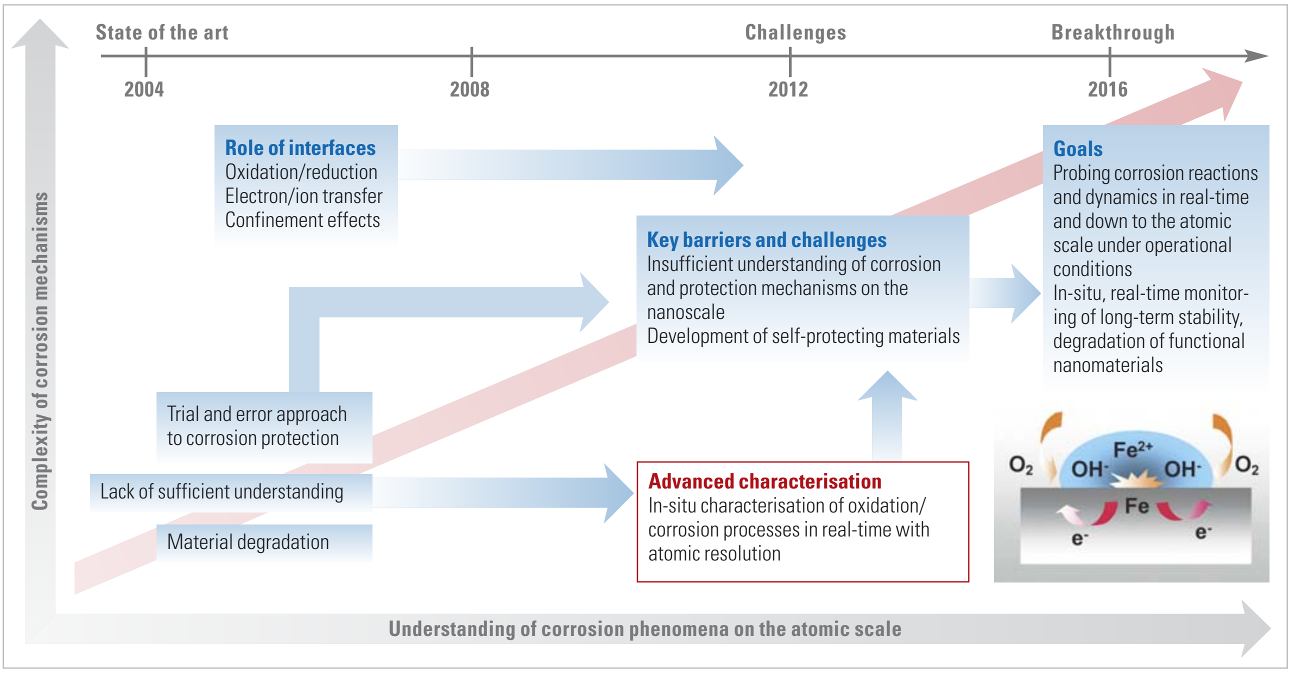

Fig. 4.3.1: Roadmap for the understanding and control of nanomaterial corrosion mechanisms and protection.

radiation and neutrons with other complementary analytical in-situ techniques, such as optical vibration spectroscopy.

- To implement combinatorial material research for corrosion studies, allowing to map the composition, pressure and temperature parameter space to provide a database for the optimum corrosion protective material in a given industrial application.

Conclusion

Synchrotron radiation and neutron large-scale facilities are ideal tools to generate new knowledge in corrosion/oxidation phenomena of nanostructured alloys which are of vital importance for industrial applications. These sources permit non-destructive structural and chemical characterisation over length scales from metre to picometre and timescales from days/hours to femtoseconds under the simulation of industrial operation conditions. This will lead to sustainable production technologies which are able to produce new corrosion-resistant materials and which can control/improve the performance and guarantee longer lifetimes of industrial plants.

RESEARCH AREA	Design of self-protecting nanomaterials	Analysis of corrosion/oxidation protection failure mechanisms	Nanopattering of large surface areas
KEY BARRIERS	Lack of non-destructive, in-situ characterisation under technically relevant oxidation or corrosion conditions with atomic resolution	Lack of in-situ characterisation of the kinetics and transient stages present during corrosion	Lack of understanding of self-organised oxidation/corrosion phenomena
FUTURE NEEDS	Understand chemical degradation mechanisms of nanomaterials in technically relevant environments on an atomic level combined with modelling of oxidation/corrosion processes through a multi-scale approach	Tailor ideal protection (self-repairing intelligent coatings; compositional gradients) for materials with longer lifetime and higher corrosion resistance	Tailor corrosion processes for large area surface nanopatterning used as templates in bottom-up technologies
SYNCHROTRON RADIATION AND NEUTRON EXPERTISE	Atomic scale, non-destructive structural and chemical in-situ characterisation of protective layers from ultrahigh vacuum to atmospheric pressures or liquid environments at elevated temperatures	Time-resolved high resolution in-situ experiments, pumpprobe experiments during oxidation/corrosion	In-situ monitoring of self-organised, corrosion induced patterning processes on an atomic level

Fig. 4.3.2: Key barriers in the field of nanocorrosion and a summary of synchrotron radiation and neutron based expertise to overcome them.

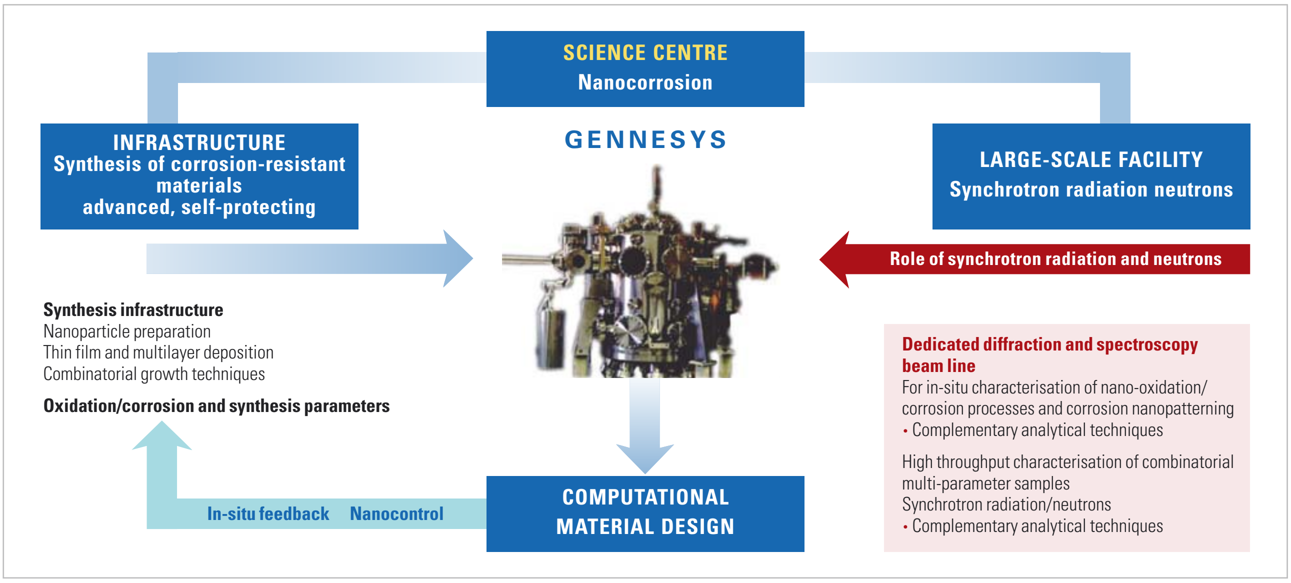

Fig. 4.3.3: Scenario for a nanocorrosion science centre interlinking preparation of corrosion resistant nanomaterials, in-situ on-line performance synchrotron radiation and neutron characterisation and computational material design.

4.4. TRIBOLOGY: FRICTION AND WEAR AT THE ATOMIC SCALE

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4.4.1. NANOTRIBOLOGY

Nanotribology is the study of friction, wear and adhesion at the nanometre scale. When objects consisting of only a few hundreds or thousands of atoms slide past each other, our everyday life picture of friction does not hold. Friction on the nanoscale usually arises from rather discontinuous processes, where contacts formed by a few interatomic chemical bonds are suddenly broken and then formed again. Nevertheless, it is extremely important to understand what happens on this scale, considering that mechanisms as diverse as the corrosion of metals and some or several human diseases start with the occurrence of unpleasant "nanotribological" events, which we would like to be able to minimise or at least control. How to do that is a formidable challenge for researchers and engineers. Friction and wear are tremendous problems on the nanoscale, which can be easily understood considering that the ratio between surface to volume forces increases as the inverse of size of a nano-object. Unfortunately, traditional liquid lubricants become too viscous when confined on molecular scales, and new ideas and methods need to be developed, like superlubricity and possible ways to achieve it.

Nanotribology is a truly interdisciplinary subject requiring knowledge of surface interactions, chemical environment effects, lubrication, mechanical stresses, as well as biochemical concepts. It is rapidly maturing, but most of the applications that can be realised exploiting nanotribological ideas are still in an embryonic stage. Fig. 4.4.1 gives an overview of current "hot topics" in this field.

What will be the practical impact of such a fascinating field of research in the near future?

- At the microscale, the ability to produce durable low friction surfaces has become an important factor in the miniaturisation of moving components in many technological devices. These include MEMS/NEMS applications, magnetic storage and recording systems, miniature turbines, many aerospace components and so on. Furthermore, the most recent development of new materials synthesis methods (such as the production of nanocrystalline materials, thin films with atomically smooth surfaces, nanoscale multilayers, nanosized clusters, and surface restructuring on a nanoscale) enables the design of surfaces, films and coatings with novel, tailor-made properties, combining the properties of the individual nanoscale compounds and making use of the interaction between them.

- These results will have a positive influence on industrial applications at the macroscale. Here, critical issues can be recognised in many of the moving parts in transportation, power generation plants, etc. Surface contacts can lead to wearing away of material, leading to failure. For moving parts, contact can cause friction and local heating which leads to additional energy input being needed in order to overcome such forces. The design and control of surface properties is also important in medical and biological applications for surface protection and lubrication layers. Surface engineering can improve the wear resistance of materials for prosthetic implants, or improve biocompatibility by providing a better surface for bone to 'key' onto.

- Last but not least, we should not forget that friction in practice seldom occurs from the solid-solid contact of two surfaces, but it is usually mediated by a lubricant system. Thus, the optimisation of the tribological properties of any mechanical system must rely on a robust knowledge not only of the surface properties of the contacting parts, but also of the lubricant layers in between. Here, nanodispersions of solid particles can provide beneficial rheological and lubricating properties to reduce energy losses in the systems and improve their performance over a wide range of operating temperatures.

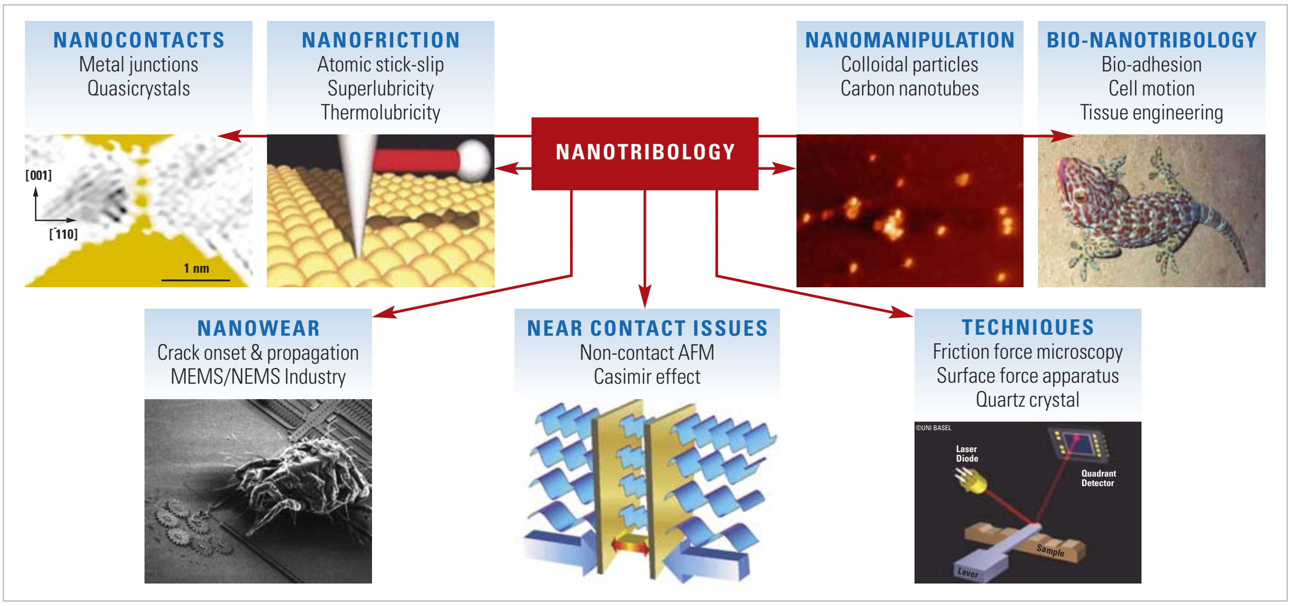

Fig. 4.4.1: Overall description of nanotribology.

4.4.2. STATE OF THE ART RESEARCH

Established twenty years ago with the observation of atomic features when two graphite flakes slide past each other, friction force microscopy currently allows tracing and controlling the motion of the smallest imaginable contacts, i.e. two single atoms sliding past each other. In clean environments like ultrahigh vacuum, different kinds of motion can be "tuned", from a superlubricated regime with negligible energy dissipation up to uncontrolled but still detectable abrasive processes. The simplicity of the systems investigated up to now made possible a fruitful interaction between experimentalists and theoreticians, which is an exception in the long history of tribology. In such a way, our comprehension of solid friction was enriched by elegant models explaining the role of thermal fluctuations, the conditions leading to superlubricity, or the distinction between photonic and electronic friction, for instance. Remarkably, most of this work was realised in Europe and/or by European scientists.

Some of the most exciting results obtained so far:

- Friction can be traced down to the atomic scale on "clean" surfaces;
- Material contrast is easily observed in frictional measurements, so that microscale friction can be used to produce "chemical mapping" of surfaces;
- Stress, temperature and humidity effects can be monitored in simple atomic force microscope (AFM) experiments;
- Friction can be "tuned" down to negligible values on the nanoscale. Various techniques have been developed, such as steady and dynamic superlubricity, structural lubricity, thermolubricity;
- Wear onset on the atomic scale has been revealed. Wear processes on the nanoscale can be traced down;
- Frictional forces acting on nanoparticles moved on a substrate by an AFM tip can be quantified; controlled manipulation of bare and coated nanoparticles and determination of dissipated energy during their manipulation;
- Molecular dynamics simulations provide important information on atomic-scale mechanisms accompanying sliding on nanometre scale.

Altogether, these and other results are summarised in Fig. 4.4.2.

4.4.3. RESEARCH TOPICS FOR THE FUTURE

Nanotribology has great potential in applications that will be made possible by a better understanding of its mechanisms and how they can be tailored in innovative products and techniques. Here we summarise some urgent requests to the growing community of nanotribologists.

Theory: Improving our theoretical understanding

- Further development of analytical models of friction and wear on the nanoscale;
- Bridging the space-time gap between molecular dynamics and continuum mechanics, and predicting how friction scales down from multi- to single-asperity contacts;
- Modelling the motion of nanoparticles driven by an external force on a surface.

Experimental techniques: Using advanced experimental methods for new nanotechnologies

- Accurate AFM experiments focusing on the role of mechanical stress, surface morphology, electric conductivity, chemical interac-

FRICTION ON THE ATOMIC SCALE
- Atomic stick-slip processes
- Friction on thin crystal films
- Dissipative channels on the nanoscale

CONTROL OF FRICTION
- Steady and dynamic superlubricity
- Structural lubricity

THERMAL EFFECTS IN NANOFRICTION
- Influence of phase transitions
- Thermolubricity

FRICTION AND ELECTRONIC TRANSPORT
- Electronic vs phononic friction
- Friction vs electrical resistivity in nanojunctions
- Tribocharging on the nanoscale

FRICTION ON NANOSTRUCTURES
- Role of nanoroughness
- Multi-asperity contacts

INSTRUMENTAL ASPECTS
- MEMS/NEMS with longer lifetime
- Ultrasonic force microscopy
- SEM/TEM applied nanotechnology

NANOWEAR
- Mechanisms of wear onset
- Wear models on the atomic scale
- Tribochemistry
- Nanoidentation
- Propagation on nanocracks

MANIPULATION OF NANOPARTICLES
- Sliding vs rolling on the nanoscale
- Mechanics of nanowires and nanotubes
- Nanoparticles as solid lubricants
- Control of nanoparticle mobility by tuning functionalisation, shape, size and their environment

BIO-ORGANIC-NANOTRIBOLOGY
- Polymer friction
- Mechanical recognition of biomolecules
- Mechanisms of cell adhesion
- Motion of viruses, bacteria, etc.
- Tissue engineering

NANORHEOLOGY
- Motion of nanodroplets
- Nanoconfinement
- Superhydrophobicity
- Boundary lubrication

Fig. 4.4.2: Main current topics in nanotribology.

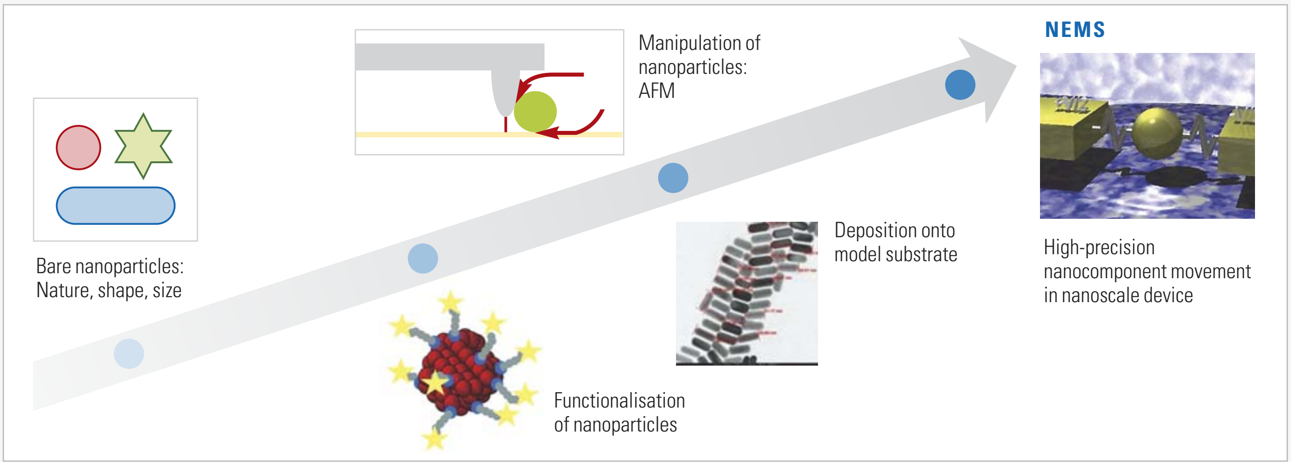

Fig. 4.4.3: Manipulation of nanoparticles for NEMS.

tions, and temperature in friction and wear processes on the nanometre scale;

- Control of friction on the nanoscale: how can we exploit the recently discovered phenomenon of superlubricity?
- Development of nanotribology in liquid environments (important for biological applications);
- Manipulation of nanoparticles: distinguish rolling vs. sliding, understanding how the motion of the particles is influenced by their size, shape, properties, the environment and their chemical coatings (see Fig. 4.4.2 and Fig. 4.4.3);
- Development of "friction-related" imaging techniques (ultrasonic force microscopy, "superlubric force microscopy").

Applications of nanotechnologies using customised nanotribology to new products and techniques

- Successful design of micro- and nano-electromechanical devices with accurate control of friction, wear and adhesion problems;
- Design of new lubricants exploiting nanotribological effects for widespread engineering applications.
- Design of self-lubricating nanostructured coatings for low-energy-loss moving and contacting parts.
- Molecular electronics: can we guide the motion of nanoparticles or even molecules in order to form a nanowire?
- Nanocatalysis: elaboration of controlled patterned surfaces (such as multiplexed assays) of functional nanoparticles to carry out novel

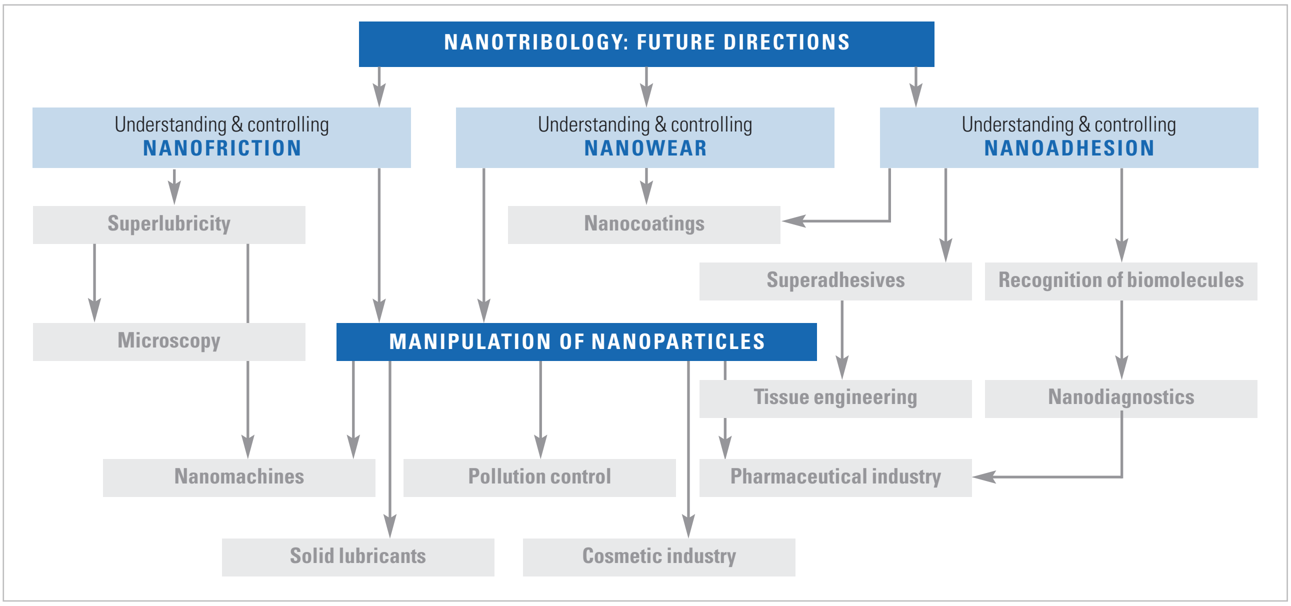

Fig. 4.4.4: Challenges for nanotribology research.

functions in biological reactions or electro-oxidation reactions in fuel cells.
- Biology: using nanotribological knowledge to understand (and control?) the motion of viruses, bacteria or blood cells.
- Medicine: formulation of new drugs by nanoassembly.
- Nanofluidics: improvement of transport, delivery of nano- or micro-volumes of fluids into nanobiological and analytical platforms or devices such as embedded biofluidic chips.
- Optics: can nanotribology contribute to revolutionising conventional optical sensors by perfectioning opto-electronic modules or improving their highly precise movements (a self-aligning system for instance)?
- Data storage applications: increase of capacity, transfer rate of nanoscale hard or flash memories?

Numerous cross-links between theory, experiments and applications of nanotribology can be imagined. Fig. 4.4.4 shows some of them and indicates some appealing directions for the future.

An outline of the research roadmap in the field of nanotribology is given in Fig. 4.4.5. The research will have two key scientific phases:
- 2007–2015: Tracing the foundations of friction and wear on the nanoscale.
- 2015–2020: Development of new nanomaterials with tailored tribological properties and nanoengineered surfaces; development of new methods and applications that are not currently achievable, ranging from engine components for cars that improve fuel efficiency, to nanomachines to be used for microsurgery and repair of the human body.

The keywords in the two phases will be understanding and, respectively, controlling friction, wear and adhesion on the nanoscale.

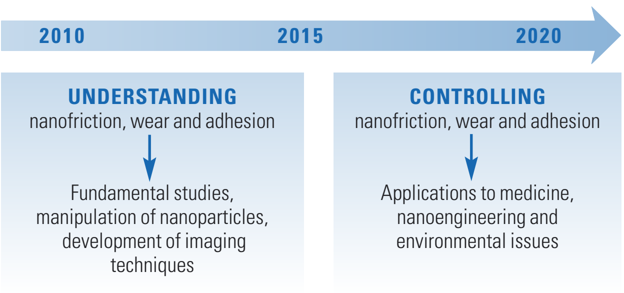

Fig. 4.4.5: Research roadmap for nanotribology.

4.4.4. ROLE OF SYNCHROTRON RADIATION AND NEUTRONS

Underpinning the topics described in the previous sections are fundamental advances arising from the application of neutron and synchrotron x-ray radiation methods to nanotribology. Synchrotron x-ray diffraction is routinely used for the analysis of the relationship between stress and strain in materials and thin films, while hard x-ray imaging and fluorescence microscopy are the techniques of choice for the inspection and analysis of local defects, homogeneity and chemical composition of engineering materials. In recent years, important developments at 3rd generation synchrotron sources have enabled the application of these techniques to systems relevant to understanding friction and lubrication at the micrometre or nanometre scale. Below we mention a few exciting possibilities, applying new understanding to the tribological behaviour of solids, foams, biological materials, colloids, emulsions and liquids. An overview is given in Fig. 4.4.6 and Fig. 4.4.7:

MATERIALS		METHODS
Solids	Optimising hardness for wear resistance and reduced friction	Diffraction
Thin organic films	Investigating the properties of collagen fibres for arthritis treatment	SAXS imaging and tomography
Suspensions	Optimising fluid composition for low viscosity	
Tissues Colloids Microemulsions	Optimisation of structure, composition and porosity	Phase contrast imaging
Confined fluids and microfluidic systems	Studying local lubrication, dynamics and flow mechanisms	Microbeam analysis and diffraction; quasi-elastic scattering

Fig. 4.4.6: Overview of the tribological behaviour of solids.

- Characterisation and understanding of effects of defects in conventional Si layers;
- Determination of inhomogeneous strain fields and local distribution;
- Measurements of stress distribution close to surfaces, grain size and average g.s. distribution;
- Microstructure (phase distribution, temperature dependent stability, porosity, microcrack formation;
- 3-D chemical elemental mapping of surfaces under wear conditions (nanostructure formation and dissolution of second phases;
- Characterise non-equilibrium states of matter induced through friction and wear/phase transformations

Fig. 4.4.7: Overview of specific topics in nanotribology.

- In-situ Laue diffraction from micrometre-sized pillars under compression, which captures changes in the material's microstructure during plastic deformation. Individual events of slip between crystal planes can be made visible. Strengthening can be observed in objects of smaller size ("smaller is stronger"). One of the long-term goals is to optimise the material's hardness. Such hardness tests are ultimately to be carried out on the nanoscale ("nanoindentation") with the use of nanometre-sized x-ray beams. This research may also help coating manufacturers in the development of wear-resistant or low-friction coatings on surfaces.

- Small-angle x-ray and neutron scattering (SAXS and SANS) from suspensions and granular materials under shear flow, with the aim to correlate the fluid's viscoelastic properties to changes in the positional and orientational correlations of the fluid's constituents. The fluid's composition can be optimised to achieve low viscosity, specific lamellar orientations, etc.

- X-ray micro- and nanotomography of colloidal suspensions, micro-emulsions, tissues, foams and granular materials. Use of x-ray phase contrast enables detailed structural characterisation of low-Z materials in foods, biomedical applications and personal care products. Structure, composition or porosity can be optimised to achieve, e.g., maximum lubrication, longer lifetime, or high absorbance. Neutron tomography can map, e.g., variations in the hydrogen concentrations and other light elements on a longer length scale, and even phase contrast imaging is possible with neutron beams.

- SAXS imaging and tomography from, e.g., thin organic films. Micrometre-sized beams are scanned over the sample and at each spot a SAXS pattern is taken. For selected spatial frequencies or orientation angles of the scatterers, images or tomograms can be constructed. One may investigate, e.g., the network of collagen-II fibres in cartilage of bones between joints with the aim of understanding the damaging effects of arthritis. This particular example of friction and wear affects the daily lives of millions of people.

- Ordering phenomena in confined fluids. The classical model of a lubricating system is a fluid confined by two opposing surfaces at nanometre distance. When the distance between the surfaces becomes less than typically ten times the molecule diameter, the lubricating properties are drastically affected. The fluid's viscoelastic properties are believed to be correlated with an ordering of the fluid's molecules in layers parallel to the confining surfaces. It is a true challenge to determine the structural properties of the confined fluid, since it requires a micrometre-sized x-ray beam to be focused onto the liquid contact region between the two surfaces. Moreover, the beam is scattered from a volume as small as a femtolitre. Such experiments, if possible, will lead to a fundamental understanding of lubrication on a molecular scale.

- Scattering from fluids in micro- and nanocavity arrays. Micofluidic systems are in use as DNA chips and more generally as 'lab on a chip'. In confinement geometries of 10–100 micrometre size, fluids start to exhibit different flow properties (laminar flow, high fluidic resistance). Confinement in arrays of even smaller sized cavities or pores (1–100 nm) results in drastically changed fluid behaviour, marked by a preponderance of electric charging effects and selective diffusion of the fluid's constituents through the pore. We note that a periodic array of cavities acts as an x-ray diffraction grating, offering unique possibilities for investigations of confinement-induced ordering phenomena, averaged over the entire ensemble of cavities.

	2010	2015	2020
ADVANCES	Improved materials design	Smart materials	MEMS and NEMS exploiting nanotribological effects
CHALLENGES	Characterising wear and frictional mechanisms at the nanoscale Design of surface structures	Understanding the origins of nanotribological properties New manufacturing technologies	Step change in nanostructural design Revolution in materials development, modelling and mechanistic understanding
ROLE OF NEUTRON AND SXR METHODS	Characterisation of: stress distribution; residual stress; grain size and distribution; elemental mapping; tomography of porosity and damage		

APPLICATIONS OF NANOTRIBOLOGICAL EFFECTS

Novel uses in medicine, electronics, MEMS/NEMS, etc.
Implants for disease control and cure

Building nanostructures	Using nanofrictional effects
· Overcoming frictional effects to move and assemble nanoparticles	· High pressures can be used to generate nanostructures "actively"
· Tailoring nanosurfaces for optimised properties	· Need to understand interaction between applied stresses, surface structures and wear behaviour
· Need real-time measurements of nanoscale interactions, which can be provided by neutrons and synchrotron x-rays	· Revolution in materials development, modelling and mechanistic understanding

Fig. 4.4.8: Applications of nanotribological effects.

4.4.5. RECOMMENDATIONS

- Reduction of friction for moving parts of engines, turbines, micromechanics, etc. to minimise exhaust and energy consumption.
- Tailored design of interfaces with reduced friction coefficient.
- Synthesis of new materials and coatings with novel tailor-made properties (nanocrystalline materials, thin films with atomistically smooth surfaces, nanoscale multilayers, nanosized clusters and their compaction, surface microstructuring on a nanoscale.
- Study of properties over various length scales and understanding mechanisms in the elastic and inelastic range.
- Development of low-friction (lubrication-free) carbon-based materials (DLC, pyrolitic carbon, graphene, nanodiamond with cof of $<< 0.1$).
- Development of new measurement techniques ranging from nanometres to large components.
- Effect of mechanical stresses/force on nanocoatings and long-term stability.

- Atomic mechanisms in friction wear.
- Effects of surface modifications due to tribology.
- Effects of plastic deformation through friction-induced large shear forces for high-speed trains, machining, cutting operations, wire drawing, shot peening and other industrial processes, for example in the field of microparts and microsystems.

4.4.6. CONCLUSIONS

- The potential impact of nanotribology is widespread. New coatings to reduce friction in vehicle engines can greatly reduce carbon emissions when applied across the millions of vehicles used on our roads. There are great prospects in the nanomanipulation of engineered particles to form new 2-D and 3-D structures, new surface properties, new drugs and new nanomachines.

  Major industries, such as the automotive industry, depend strongly on innovation. One important development is the incorporation of novel materials with reduced weight, e.g., aluminum or ceramics parts, where the tribological understanding is lacking. The tools of nanotribology will help to overcome these problems. A second class of industrial applications is related to MEMS, where one expects a variety of new devices in the field of non-invasive microsurgery. Here, the central problem is the life-time of micromotors, which has to be increased.

- Order of magnitude size reduction of microsystems for: magnetic storage and recording systems, miniature motors, aerospace components, microfluidics, biolabs.

- Reduce energy consumption and exhaust by 30% in transport systems (green car concept) by 2020.

- In order to obtain benefits from research investment in these areas, there will be a need for highly-skilled professional "nanoscientists" and "nanoengineers", who are educated in the physical and engineering fundamentals and have expertise in applying advanced experimental techniques, particularly using neutron and synchrotron x-rays.

- A central focus for nanotribology research will be needed in order to bring together researchers, instrument scientists, experimentalists and engineers with the right combination of skills and expertise. The formation of a European Centre of Excellence in Nanotribology (ECNAT), integrating expertise from across Europe, will provide the impetus and the capability for capitalising fully on research investment in these areas.

- ECNAT will be sited at a major research facility, housing materials characterisation, prototype process plant, and having close access to neutron and synchrotron x-ray beam lines. The institute will host a world-leading research effort into nanotribology mechanisms, effects and applications. In addition to dedicated research and support staff, the centre will take a lead in training the next generation of international researchers by hosting a large cohort of research students; and will operate a prestigious visiting fellowship scheme to enable scientists and engineering based in industry to contribute to and benefit from leading edge nanotribology research. The Institute will also work to provide training materials for technical staff based in industry to help them engage with new methods, techniques and applications.

4.5. JOINING OF NANOMATERIALS

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The rapid growth of nanotechnology research will only prove useful when the nanomaterials produced can form integrated parts of devices and components. Nanojoining technology driven by present needs (Fig. 4.5.1) will be the key factor in enabling quantum leaps in technological advancement.

In order to achieve the complex potential and to take advantage of the full impact on the development of nanomaterials, joining must turn into an integral part of primary processing (Fig. 4.5.2), into a process which creates desired structures and is practised as much by physicists as by welders. Synthesis of nanomaterials, device and assembly need to occur in the near future as an integrated and preferably simultaneous procedure. Besides the development of new joining concepts, a comprehensive treatment of joining in research and in education has become indispensable.

This section addresses some of the expected challenges, future vision, research road map and impact of dedicated neutron and synchrotron radiation tools related to nanojoining methods.

Challenges: Nanojoining and industrial potential (Fig.4.5.3)
Structural applications: In this context, nanojoining refers to the methodology of joining high-strength nanostructures without deteriorating the nanostructure achieved during the original synthesis. The development of novel joining concepts will satisfy the current needs of business and social needs with reference to automotive, aerospace, chemical, energy, medical and microelectronics industries.

Electronics and photonics: Nanojoining will take the key role to reach the breakthrough in miniaturisation behind Moore´s law. The critical issue is the manipulation of structures as a function of constitutional elements and external field variables to induce joining and obtain the intended electronic and optoelectronic properties. Special joining techniques and methods are required to enable MEMS or NEMS assembly. "Self-forming joints", self-limiting joining, "self-assembling structures" are currently under intensive development.

Molecular electronics: Molecular electronics has attracted a huge interest in researchers trying to develop new miniaturisation strate-

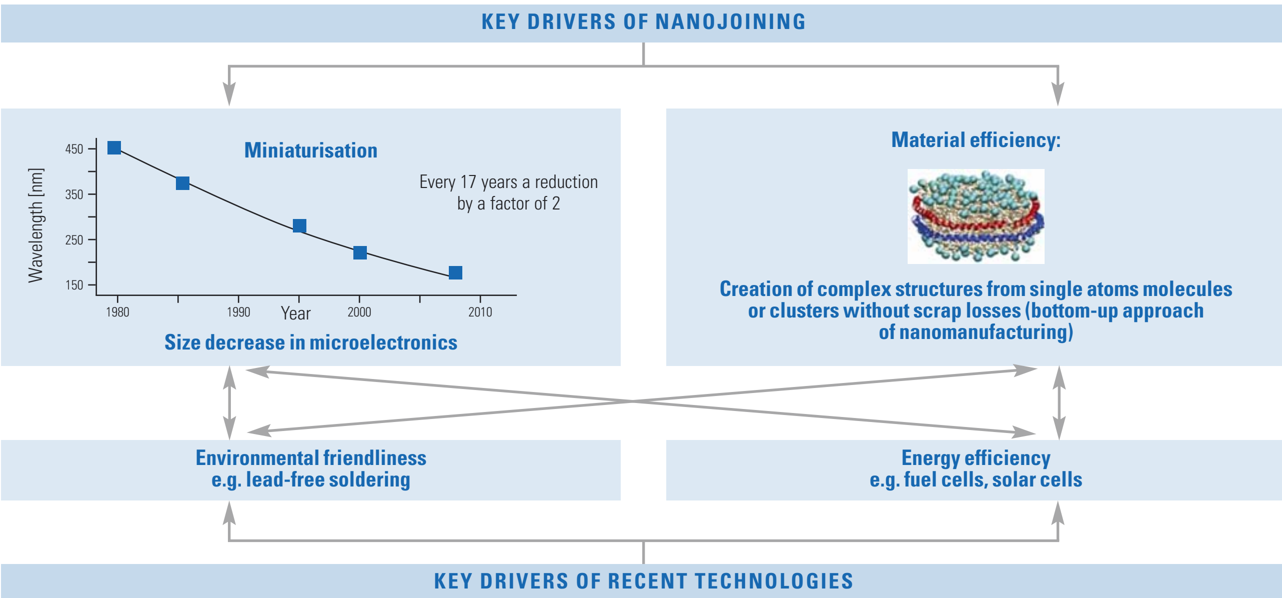

Fig. 4.5.1: Main key drivers of nanojoining technology.

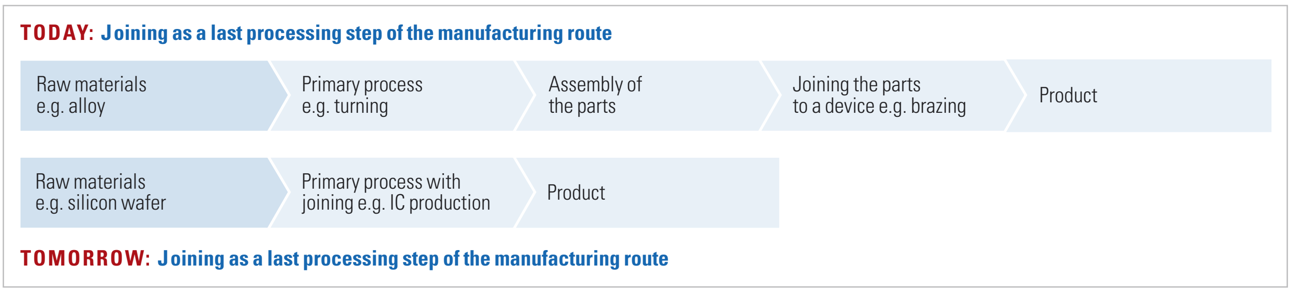

Fig. 4.5.2: New role of the joining process.

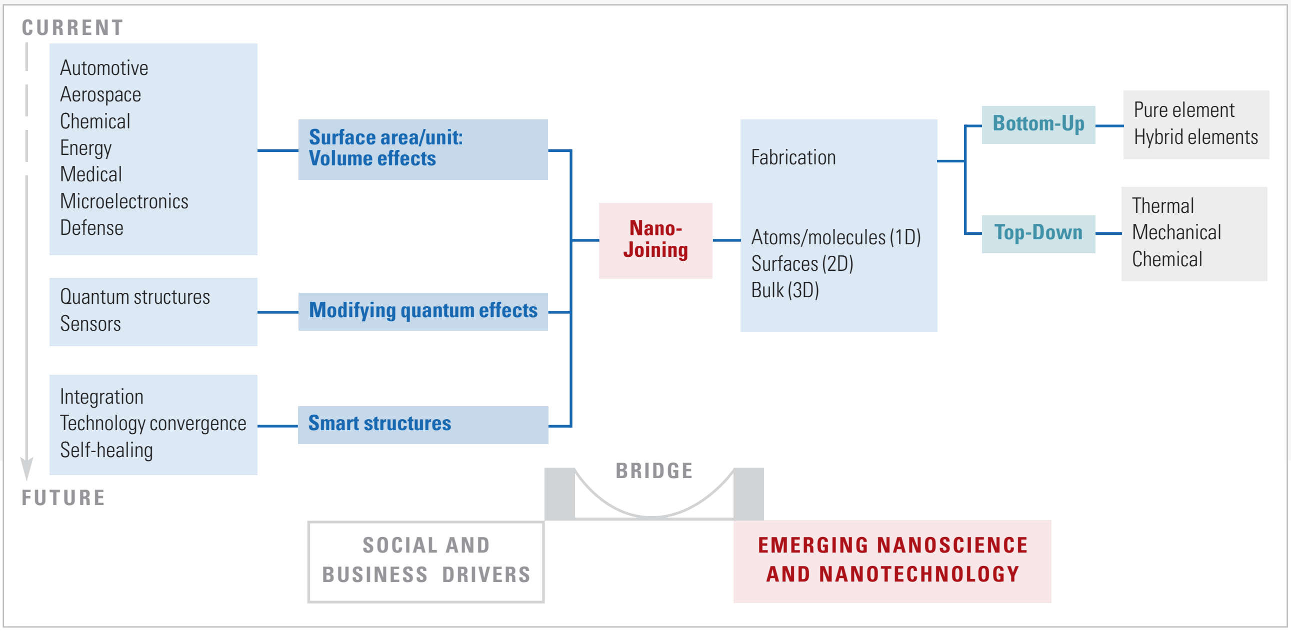

Fig. 4.5.3: Overview of the importance of nanojoining for current and future applications.

gies in the electronics and computer industry. However, production of single molecule devices has remained a challenge because of the difficulties in achieving electrical contact between individual molecules. The advent of carbon nanotubes has raised some hopes of achieving this goal.

Smart structures with integrated technologies: Only the development of robust nanojoining technologies without influencing their quantum effects, it becomes visible to design and fabricate smart structures with embedded sensing and actuation systems, as nanoscale materials/devices with different sensitivity to different molecules/threats with an on-board communication module to a large-scale counter thread device.
All these conceptual designs can only be achieved by a fundamental understanding of physical, chemical and biological interactions during and after joining of these nanomaterials. There is an urgent need to develop multi-scale computational models that can predict the performance of these nanostructures by considering the quantum effects as a function of composition (silicon or carbon based), size and external field (pressure, temperature, substrate, magnetic field etc).

2. State of the art: Research on nanojoining

The area of nanojoining can be divided into three groups: joining of nanomaterials, joining with nanomaterials and forming nanoscale joints (Fig. 4.5.4).

Joining of nanomaterials

The aim of joining nanoparticles and structures with special functional properties (nanomaterials with high electrical and thermal conductivity, i.e. carbon nanotubes) is on deliberate joints with a desired func-

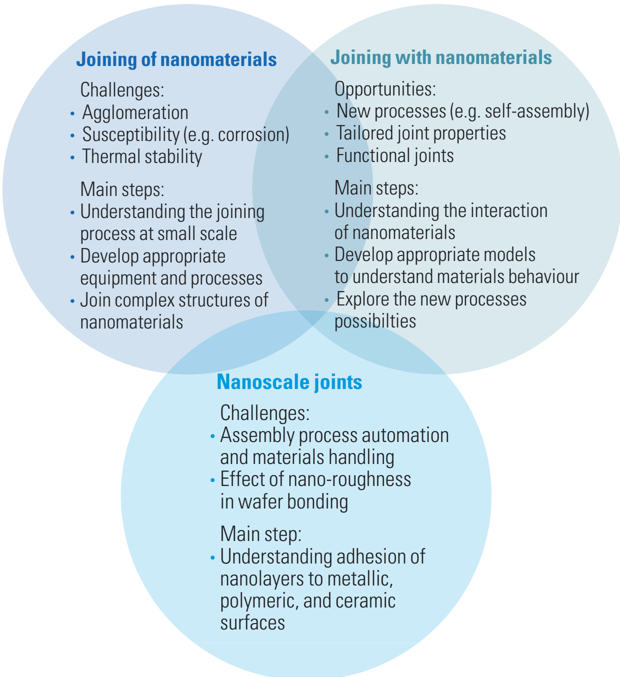

Fig. 4.5.4: The activity fields of nanojoining.

tionality; this is particularly important in the future of electronics. The usually problematic tendency of nanoscale materials to agglomerate and stick to each other due to their high surface areas can be used to create self-assembled joints in nanoparticles. Use of power beams (electron beam, laser and ion beams) has been reported to join nanowires and nanotubes.

In the joining of bulk nanomaterials, the poor thermal stability of nanomaterials excludes the use of the most conventional joining (e.g. heat activated processes) and requires the development of new joining concepts. The research is directed onto powder metallurgy, diffusion bonding using nanomaterials at the interface, electrodepositing metallic nanocoatings on other nanostructured materials, exothermal brazing and gluing.

Joining with nanomaterials
The known melting point suppression of nanoparticles can be utilised to significantly reduce the joining temperature and to minimise thermal stresses during processes. This may bring a short-term solution for current problems of lead-free soldering technology especially in the higher temperature range applications.

The shortening of the diffusion distances when using nanosized joining media can reduce the processing time from hours to minutes or even seconds, turning the laboratory processes into potential industrial processes. Especially environmentally-friendly joining concepts may be developed in this way.

Applied to the process of self-propagating high-temperature synthesis (SHS), the size effects allow initiating the exotermic reaction at room temperature. Those results are a very important opportunity for a "cold" joining process that would be gentle to the nanostructured materials whilst joining (e.g. room temperature fluxless soldering IC packages or component mount onto printed circuit boards).

Optical properties of nanomaterials can be fine-tuned according to their sizes to achieve energy efficient joints using power beams. Nanomaterials can also be used to impart functionalities into a joint including thermal or electrical conductivity, mechanical enhancement or ease of disassembly and recycling.

Forming nanoscale joints
The tailored design of nanojoints is one of the many ways to preserve and use all the unique properties of nanomaterials integrated into current technologies. Processes used to achieve refined interfaces to include nanosized structures with enhanced properties have to be developed. This also includes coatings and adhesion of nanolayers to metallic, polymeric and ceramic surfaces, e.g. wafer bonding.

Future vision (Fig. 4.5.5)
The future of nanojoining can be envisioned in four distinct steps:
- Extensive efforts related to multi-scale nanomaterials;
- Efforts to correlate the nanostructures to their inherent physical and chemical properties and to develop a fundamental understanding of the joining process;
- Transformation of this fundamental knowledge on nanojoining into multi-scale computational models. These efforts will also lead to methods to sense and control the spatial location of these nanostructures either through external fields or by self-assembly mechanisms;

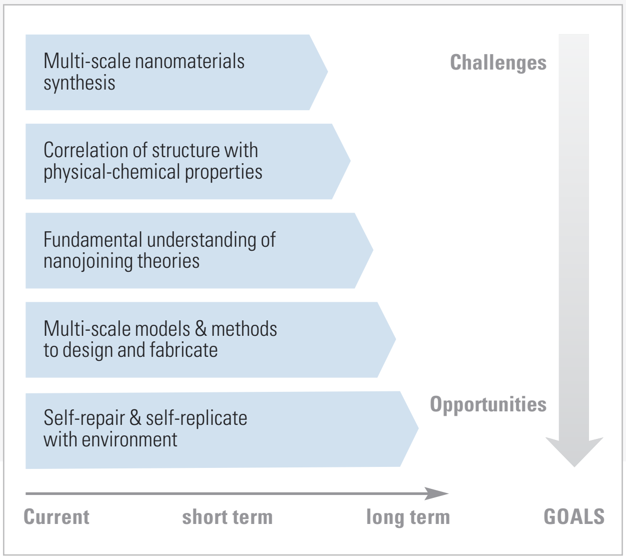

Fig. 4.5.5: Vision for the role of nanomaterials joining in the context of nanomaterials applications. The uncertainty in predictions increases with time.

- Development of a strategy which allows to design a set of nanoscale materials on a computer and download the synthesis and joining procedures in order to obtain a structure or device for particular application.

Research roadmap
It is important to note that there are many scientific and technological challenges that need to be addressed to meet the proposed future. A short- and long-term research roadmap is described below briefly.

Short-term goals
Important short-term applications are stressed as examples. The outcome of these short-term goals will provide the needed credibility to invest in long-term research on nanojoining.

Joining of carbon nanotubes
There is a strong relationship between structure and electronic properties of carbon nanotubes (CNTs) and this can be exploited to make electronic devices if we are successful in joining CNTs. If we can control the chirality and diameter of CNTs and can make defect-free joints, we can develop nanoscale electronic devices. For example, by joining two CNTs with different chirality, a diode can be produced; a transistor can be produced by appropriate joining of three CNTs. Innovative and reproducible joining technology needs to be developed without introducing defects in these nanotubes for the two configurations shown in Fig. 4.5.6.

Dry adhesive bonding using nanostructures
Development of conductive packaging interconnects. This technology would create a new electronic assembly process that no longer

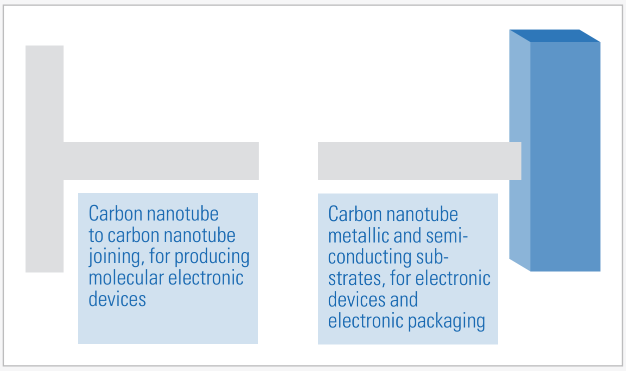

Fig. 4.5.6: Possible configurations expected for joining carbon nanotubes.

needs a solder and is performed at room temperature. It would allow paper and textile electronics high-strength assembly and create ultra-thin flexible IC manufacturing that would replace traditional plastic packaging.

- "Nano attach" technology based on biomimetic approaches (example "gecko foot") will lead to a room temperature process for streamline manufacturing and thus cause a paradigm shift in assembly.

Carbon nanotubes hooks (nanohook assembly) are realised by the substitution of hexagonal structures with heptagon-pentagon structures.

The self-assembly method is likely to be important for future large-scale production, but nanomanipulation will be probably a key technique to test prototypes and individual structures before developing self-assembly processes to mass produce these devices.

Joining of nanocrystalline alloys

Nanocrystalline alloys offer excellent material properties like high strength and superplasticity. However, joining using conventional methods like fusion joining would lose some of the properties of the base material at the joint due to grain coarsening from the heat of joining process. A novel method of joining nanocrystalline alloys therefore remains a challenge.

Joining of nanocomposites

In the automotive industry, nanocomposites are expected to replace more expensive materials, increase production, and facilitate weight reductions. Nanocomposites manufactured with commodity plastics are predicted to be the most widely used. Although nanocomposites provide promising advantages like high strength and specific density, joining of nanocomposites using conventional methods is not very well developed, and typically strength is lost at the joint. There is a high demand for joining methods that would produce consistent high strength nanocomposite joints. Initial experiments with hot plate, vibration, and ultrasonic welding have found that welding polymeric nanocomposites results in a significant decrease in weld joint strength compared to the unfilled polymer. Studies on the weldability of thermoplastic nanocomposites should continue until acceptable weld strengths are discovered.

Long-term goals

The development of nanomaterials to meet the needs of society in the future will rely on a complete understanding of the physical, chemical and biological properties of these materials.

In order to address joining of these nanostructures, it will be necessary to characterise these structures as a function of processing steps. The inherent properties may vary spatially and temporally due to quantum and size effects. A long-term roadmap to address this need is shown in Fig. 4.5.7. Focused efforts as a part of these four major categories are described briefly below.

In-situ time and spatially-resolved characterisation

In order to succeed in the joining of nanomaterials, it is necessary to understand the behaviour of nanomaterials and structures made from nanomaterials from both nano- to macroscales and different time-

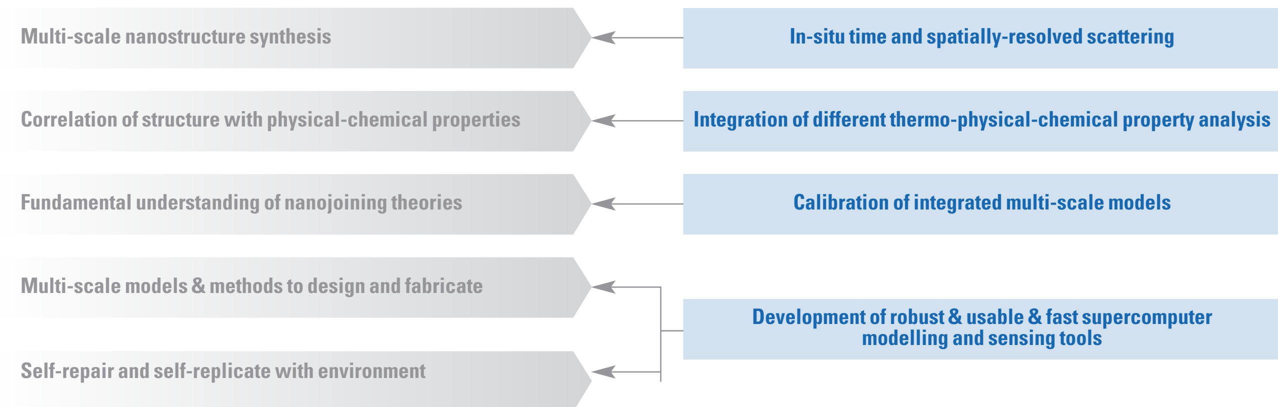

Fig. 4.5.7: Long-term research goals related to nanojoining science and technology development.

scales. Characterisation speeds may reach the upper limits of the available detectors. Innovative detection methodologies in transmission electron microscopy, synchrotron radiation and neutron techniques have to be devised and combined with other macroscopic characterisation tools (as differential thermal analysis and optical sensing.

Thermophysical- and chemical property analyses

Due to the inherent nature of the size, the thermophysical- and chemical properties of these nanostructures may become very difficult to measure using conventional techniques. Innovations in the development of nanoscale measurement devices which can interrogate newly processed nanostructure materials are warranted. These analysis techniques need to evolve parallel to integrated multi-scale computational models.

Future of nanojoining system concept (Fig. 4.5.8)

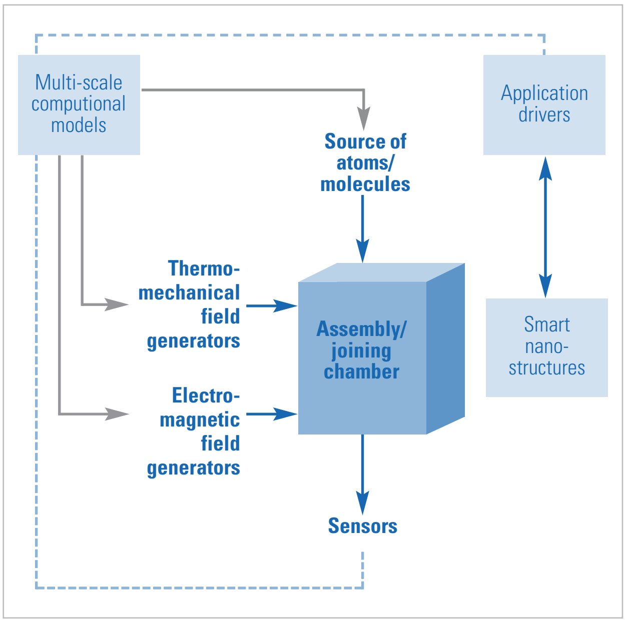

Fig. 4.5.8: System based view of future nanojoining technology.

The application drivers will lead to a conceptual design of smart nanostructure architecture. This design will be downloaded to a multi-scale computational model that is capable of setting the needed parameters for the source of atoms and molecules, thermal and mechanical field generators, and electro-magnetic field generators. The materials and processing will occur in a controlled environment chamber as series of sensors monitor the evolving structure. The sensors constantly provide feedback on the intended quality of the evolving structure. If there is a departure from the intended structure, the computational models devise methodologies to correct the defects and also drive the source and field generators to make the intended remedial action.

Future role of synchrotron radiation and neutron facilities

Although the above roadmap provides a compelling vision, there are many scientific and technical challenges that need to be addressed:

Feasibility of sensing in different length and timescale:

The system level approach calls for an ability to sense the nanostructure architecture while processing. The processing times are expected to be ranging from 10 – 9 seconds to 102 seconds depending upon the complexity of the structure. The gradients in these structures may be in the scales of 10 – 10 m to 10 – 8 m. The overall structures that need to be fabricated may be in the range of 10 – 8 m to 10 – 6 m.

Feasibility of field generation in different length and timescale:

Similar to sensing, the challenge exists to control the thermo-, mechanical, electrical and magnetic fields in nano- and micron scales. These fields should be controlled only to fabricate without destroying the underlying structures.

State-of-the-art synchrotron and neutron beam lines can be used to meet the above challenges of tracking atoms and their locations as the nanostructure joints evolve.

Ex-situ 3-D characterisation of nanostructure joints (0 to 5 years)

Using the current synchrotron radiation and new neutron beam lines and new-generation of neutron beam lines, it is possible to interrogate the gradients in chemistry, structure and defects that occur in nano- to micron-scale during joining processes. It is possible to obtain a post-processed state of these structures by performing ex-situ analyses in different stages of joining processes. These characterisations can be complemented by other ex-situ characterisation techniques like high-resolution transmission electron microscopy. One of the candidates for such characterisation is to quantify the nanostructure evolution at the joints made in new generation of lithium-ion batteries to evaluate the material behaviours in different length scales and geometry. There are some emerging activities within the US, Europe, and Asia which is in alignment with the above research roadmap.

In-situ 3-D characterisation of nanostructure joints (5 to 10 years)

For a detailed understanding of joining processes there is a need to improve the spatial resolution (nanometres) and timescale (<10 – 4 seconds) and to track different lattice configurations and any change in element concentrations. The challenge will be to develop detectors and also analytical tools to interpret these measured data quickly. This requires dedicated synchrotron radiation beam line and supercomputing technologies to interpret the data on the fly during processing and experimentation.

Development of converging analytical tools (10 to 15 years)

In order to follow all the physical and chemical processes that occur during nanojoining, an analytical strategy based on different techniques such as x-ray photoelectron emission, Raman spectroscopy, Fluorescence Spectroscopy, and ultrasonic wave scattering based methods. To achieve this vision, we will require close collaboration between materials science expertise and beam line expertise.

Joining of nanostructures using high energy synchrotron and neutron beam lines (10 to 30 years)

It should be investigated, whether high-energy x-ray and neutron beams can be utilised to induce joining at nanoscales. By toggling between characterisations and processing route, a precise joining of nanostructures could be realised. To achieve this technology, the science of radiation damages on small-assembly of nanostructures with different elemental constitutions needs to be understood. This will require close coupling between multi-scale computational models for nanostructure processing and beam line designs

General conclusions and European Research Strategy

Nanojoining is a critical technology that will allow for the rapid deployment of nanomaterials for use in society. The roadmap described earlier in this section describes how nanomaterials can indeed be rapidly implemented in everyday-life applications. Unfortunately, the developments of nanojoining concepts are stifled by a lack of fundamental understanding of physical and chemical processes at these small scales. The joining challenges are described for three classes of nanomaterials i.e., based on the surface area effect, quantum effects and combinations of both. The quantum effects may lead to a completely new paradigm of modifying the joining procedure on the fly with the aid of multi-scale material models, innovative sensing and control methods (Fig. 4.5.9). The need for the use of in-situ and ex-situ tools including synchrotron and neutron scattering are stressed to develop this integrated approach for joining a wide range of nanostructure materials.

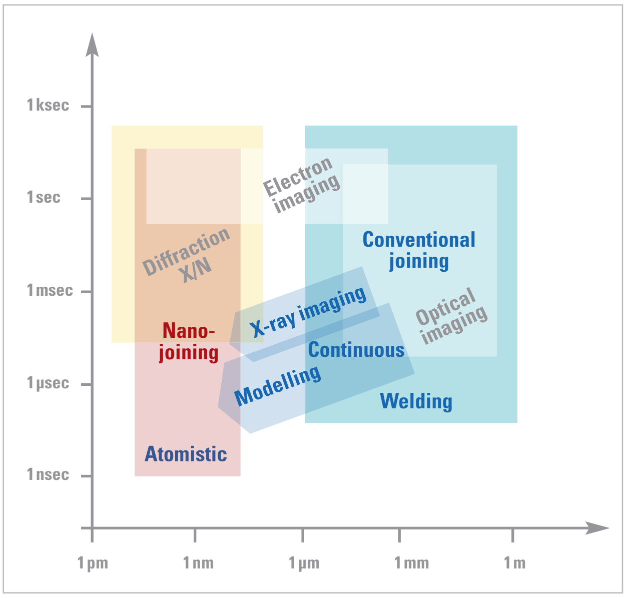

Fig. 4.5.9: Development of nanojoining concepts on the fly with the aid of multi-scale material models, innovative sensing and control methods.

4.6. METALLIC GLASSES IN NANOTECHNOLOGY

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When a conventional liquid alloy cools down under nearly equilibrium conditions, it solidifies into the lowest energy state structure and forms a coarse-grain crystalline structure, i.e. rather than forming a perfect single crystal (most metallic alloys are polycrystalline, with grains of varying shapes and sizes). Here, grain boundaries represent weak places of less than optimal atomic packing, where fractures and corrosion start. As a result of dislocation motion, metals have a much lower strength than their theoretical one and deformation is plastic. On the other hand, glassy and nanocrystalline materials are strong and hard and their strength approaches the theoretical limit. Nanometallic glasses combine superior properties and features of glassy and nanostructured materials:

- Hardness (desirable e.g. for surface coatings);
- High mechanical strength (several times that of steel but lighter);
- Toughness (more fracture resistant than ceramics);
- Elasticity (high yield strength and fully elastic);
- High atomic diffusivity;
- Soft magnetic behaviour.

Research needs

Nanometallic glassy micro- and/or nano-electromechanical systems (MEMS/NEMS) – Near net-shape fabrication methods.

Nanotechnology is an emerging frontier for the development of various future devices. Micro-and/or nano-electromechanical systems (MEMS/NEMS) are the basis of future nanotechnologies, because they combine miniature sensors and actuators with electronics. Materials selection for MEMS/NEMS fabrication is based on the careful consideration of a material's properties with regard to its intended application: i.e. many MEMS devices, such as pressure, chemical and bio-sensors, rely on actuation of a membrane structure and require a high fracture toughness material for the enhanced durability and shock resistance. On the other hand, for fabrication of controlled nanostructures, the material should be machinable up to atomic level.

Currently, the materials used for MEMS/NEMS fabrication are based on silicon or oxides, which are brittle and have size effects such as lattice defects, anisotropy, grains and grain boundaries. These effects are the limiting factors in the reduction of pattern size, especially when a dimension of the pattern approaches a few tenths of a nanometre. Considering the above-mentioned facts, one can use metallic glassy samples for the fabrication of 3-D micro-/nanostructures. Metallic glasses are known to be homogeneous, isotropic and free from the above-mentioned defects, which result from the crystalline nature. They possess very high strength and material functions such as magnetism or corrosion resistance at room temperature.

They have fundamentally glassy structure and exhibit a Newtonian viscous flow in a certain temperature range, known as super cooled liquid region. The polymer-like formability of bulk metallic glasses (BMG's) in their super cooled liquid region is already utilised for the fabrication of 3-D microstructures. As such, Bulk Metallic Glasses have the potential to replace silicon in MEMS. For example, glassy Al_3Ti-based hinges are the basis for the rotation of the micromirrors in digital light processor (DLP) technology.

Nanometallic glassy (BMG) materials, nanowires and nanocomposites as a new class of functional materials

Metallic glassy nanowires were spontaneously created on the fracture surfaces that were produced by a conventional mechanical test. The presence of the nanowires is directly related to the one-dimensional meniscus configuration with a small viscosity at high temperatures and to the wide supercooled liquid region of the metallic glass. In addition, we found that round ridges are constructed from nanotubes. The finding of amorphous nanostructures not only provides a fundamental understanding of fracture processes but also gives a new insight into nano-engineering applications.

The preferred disordered structure indicates that the metallic glass nanowires possess better structural stability under mechanical loading than the crystalline ones. Metallic glassy nanowires might be interesting objects for a wide range of applications including microwave devices, recording media, magnetic or chemical sensors, nanobiotechnology, field or light emission, tips for atomic or magnetic force microscopy.

Metallic nano-glassy composites for MEMS/NEMS

Metallic nano-glassy composites with a crystallite size of 1-10 nm were produced by tailoring the composition of metallic glasses and solidification conditions. New bulk metallic glasses have a structure different from conventional metallic glasses and possess a high degree of medium range order which explains their high relative density comparable with that of crystalline counterparts. In some cases, nanoglassy composites were produced either by direct solidification or by heat treatment in the supercooled liquid region. Such composites containing nano-icosahedral structures possess higher strength and hardness.

Magnetic nanometallic glassy materials

In order to improve soft ferromagnetic properties, one can tailor the composition and optimise the microstructure. The magnetic coercivity (Hc) is roughly inversely proportional to the grain size for grain sizes exceeding 0.1 m (where the grain size exceeds the domain wall thickness). In such cases grain boundaries act as impediments to domain wall motion, and thus fine-grained materials are usually magnetically harder than large grain materials. Recent developments have led to the conclusion that for very small grain sizes less then 100 nm, Hc decreases rapidly with decreasing grain size. This can be understood by the fact that the domain wall, whose thickness exceeds the grain size, mean that fluctuations in magnetic anisotropy on the grain size length scale are irrelevant to domain wall pinning. This important concept suggests that nanocrystalline and amorphous alloys have significant potential as soft magnetic materials.

An overview of potential use of nanometallic glasses for nanotechnology is given in Fig. 4.6.1.

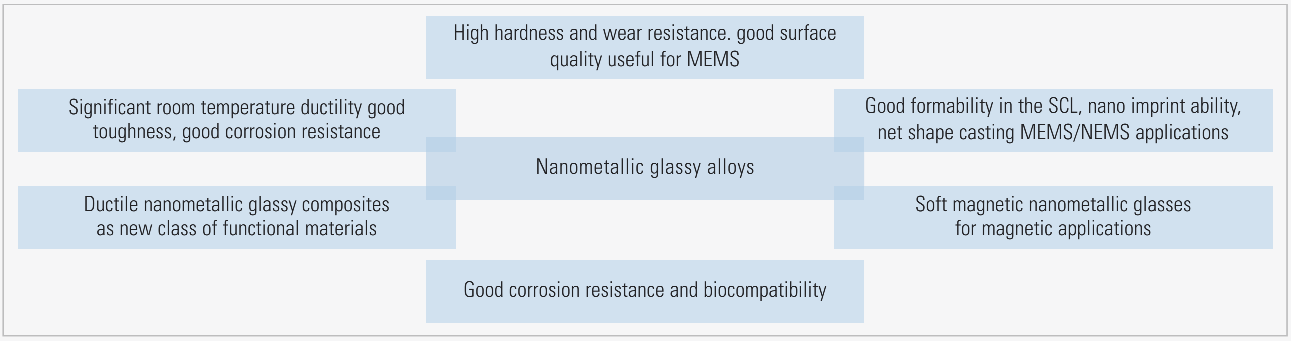

Fig. 4.6.1: Potential of nanometallic glassy materials for nanotechnology.

Tailoring of properties

In general, relatively little attention has been paid to the free volume of glasses, although it is well known that the properties of glasses depend strongly on their free volume. Depending on the preparation procedure, the free volume may be tailored in controlled ways. As many properties of glasses depend on their free volume, nanoglasses are expected to exhibit new mechanical, electronic, optical, thermodynamic, chemical properties. The basic idea to generate glasses with enhanced free volume is explained schematically in Fig. 4.6.2.

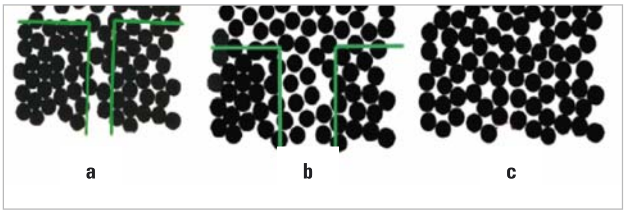

Fig. 4.6.2: The images show (in a two-dimensional model) the atomic structure of a shear band in a metallic glass (a). Upon annealing below Tg, these shear bands start to delocalise (b,c).

Future research needs

- To carry out atomic level characterisation of such materials, especially used in MEMS/NEMS applications in order to verify structure and structural stability, and thus, durability of such materials. Methods include x-ray diffractometry, transmission electron microscopy, 3-D atom probe and other methods.
- To investigate the difference in the structure between conventional marginal glass-formers and bulk metallic glass-formers which possess a high degree of medium-range order, form dense local structures and have a high relative density;
- Shear band propagation can enable plastic deformation and surpass the inherent limitations of metallic glass. Therefore, the search for advanced ductile nanometallic glasses and composites with good mechanical properties is a very timely research subject.
- To develop nanometallic glasses with good magnetic properties: high magnetisation and low coercivity;
- To characterise the structure – mechanical properties relationship of new metallic nano-glassy composites produced by tailoring the composition of metallic glasses and variation of solidification conditions;
- To produce a new generation of ductile nanometallic glasses in other systems: Cu-based, Ti-based and Ni-based;
- To study the atomic structure, free volume and the deformation behaviour by synchrotron radiation x-ray diffraction;
- To evaluate the formation behaviour of nanowires and micron-size nano-glassy samples compared to 2- and 3-dimensional nanometallic glasses;
- To develop computer modelling – powerful tool – in designing nanometallic glassy alloys in the complex systems, in understanding the role of MRO in the deformation behaviour of nanometallic glassy materials and the molecular dynamics simulation of the structure changes on cooling;
- To explore new applications of nanometallic glassy materials; important task for these fascinating materials with a very high potential for new innovations.

The research procedure is schematically shown in Fig. 4.6.3.

Role of synchrotron radiation and neutrons

The structure of nanometallic glasses is normally measured by conventional XRD and high-resolution TEM. However, synchrotron radiation is a very powerful technique to be used for structural investigation. This technique allows us to obtain local atomic information and reconstruct the structure of the material using radial distribution functions RDF(r) and partial pair distribution functions PDF (r). Moreover, structural changes, thermal expansion and free volume changes can be studied in-situ.

Nanometallic glasses can also be produced by introducing interfaces into metallic glasses on a nanometre scale which can delocalise upon annealing when free volume associated with these interfaces increases the volume of the glass. Synchrotron radiation is a powerful tool to investigate in-situ free volume annealing upon heating.

Surface nanocrystallisation can likely be achieved by shot preening treatment. This treatment is found to change the structure of the surface layer and cause ductilisation of metallic glasses by formation of the shear bands. Such structural changes in volume of a glass can be tested by synchrotron radiation.

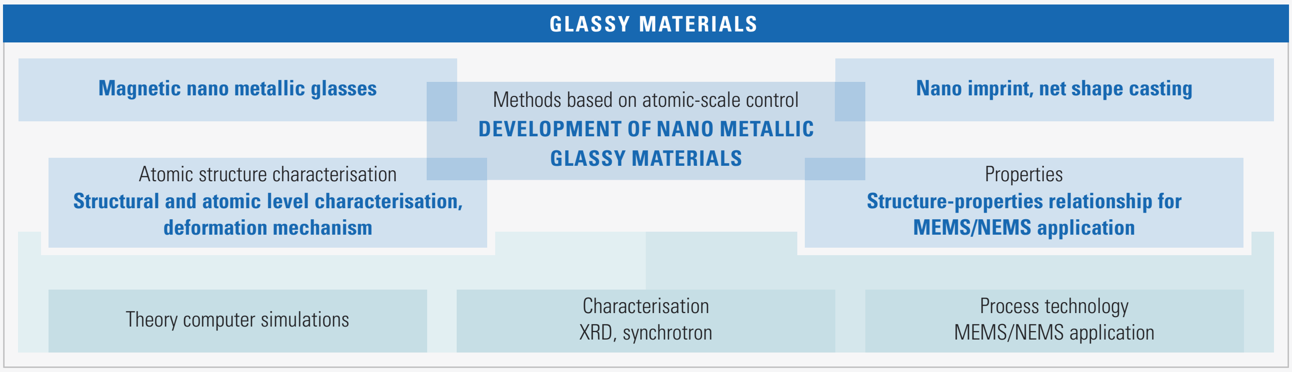

Fig. 4.6.3: Diagramme indicating the investigation procedure.

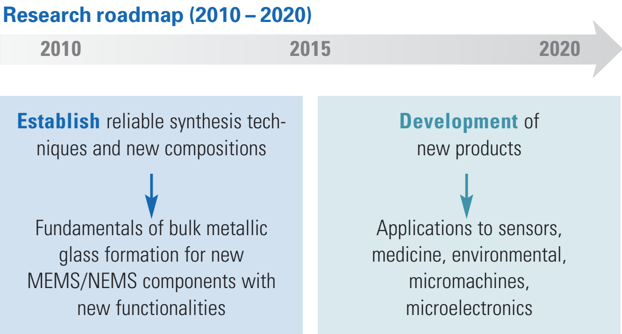

Fig. 4.6.4: Research roadmaps for nanometallic glasses.

The following topics can be studied:

- Structural characterisation of nanometallic glasses with tunable short and medium range order;
- Free volume of nano-glassy materials;
- Deformation mechanism of nanometallic glasses;
- Nanocrystallisation behaviour, in-situ studies;
- In-situ studies of deformation and fracture;
- Neutron scattering experiments for alloys containing chemically similar elements or elements having close atomic scattering factors.

Conclusion: International research

Fundamental investigations in the field of nanometallic glasses is a pioneering international research need, combining efforts from the viewpoint of structural characterisation, properties and application of such fascinating materials. It is important to develop new fabrication and processing methods for metallic glasses: bulk metallic glasses and nanometallic glasses. Sophisticated equipment like 3DAP and synchrotron analysis will be required as well as qualified personnel to analyse the data obtained. Computer modelling and structure simulation is required for the understanding of the local atomic order in such materials. These studies will widen the area of applications of nanometallic glassy materials and benefit mankind and improve technology, standards of living and prosperity of humanity.

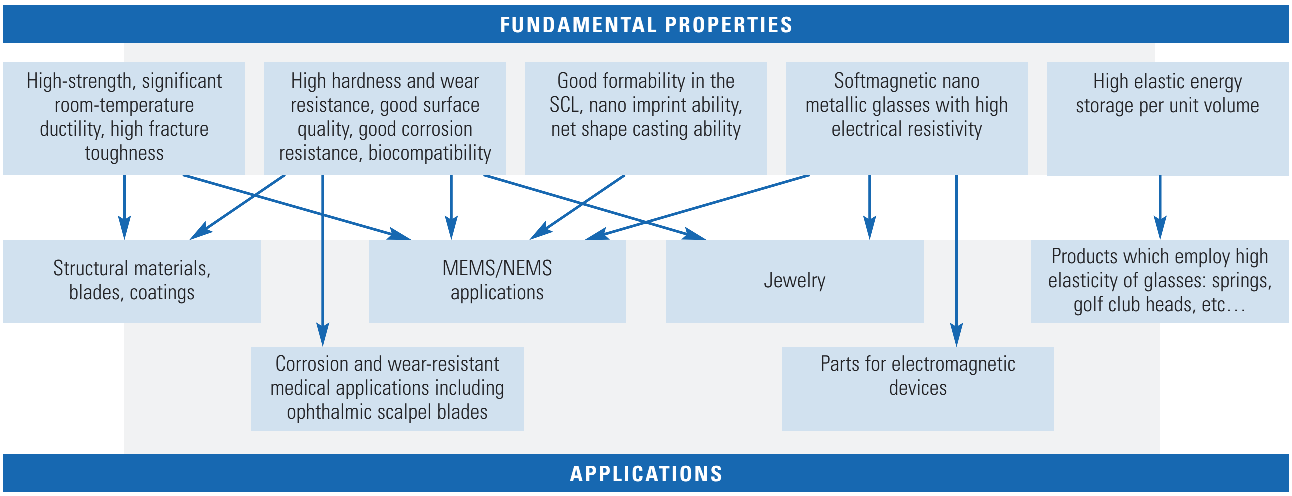

Fig. 4.6.5: Diagramme illustrating the fundamental properties and important applications of nanometallic glasses in the frame of an international collaboration.

4.7. DIRECTIONS FOR NANOMATERIALS ENGINEERING RESEARCH

AUTHORS: H. Dosch, M.H. Van de Voorde
[Affiliations chapter 12]

A number of elements are highlighted in which synchrotron radiation and neutrons are currently playing a vital and/or unique role in the prosperous developments of this new nanoengineering field.

- **Nanomechanics and nanocorrosion knowledge base**

Studies of strength, fatigue, and fracture properties at the nanoscale will require a new set of tools for their characterisation i.e. synchrotron radiation and neutrons.

In-situ testing/monitoring under various loading (i.e. mechanical stress: creep, high and low temperatures, cyclic loading: low and high cycle fatigue, etc.) conditions allows the study of phenomena such as micro/nanostructure instabilities, and subsequently offers an understanding of fracture, deformation and degradation mechanisms of nanoengineering materials.

High resolution in space results in a detailed understanding of the relationship between structure, defects, microstructure instabilities, and mechanical/corrosion degradation processes.

Synchrotron radiation and neutrons will play a key role in nanomaterials engineering studies such as the:
- Mechanical behaviour at the nanoscale with respect to the elastic, visco-elastic, plastic and fracture behaviour of bulk nanostructured materials and surfaces;
- Studies of nanoscale mechanical contacts with respect to adhesion, friction, wear;
- Nanofluids and mechanics at solid-liquid interfaces including wetting processes;
- Development of "design rules" for the preparation of new nanostructured materials and devices;
- Long-term stability of nanomaterials in industrial simulating environments: mechanical and corrosion.

Only synchrotron radiation and neutron methods have the potential to provide novel insights in the evaluation of friction at atomically smooth surfaces in real service environments. The targets for future research on nanomechanical engineering, corrosion and tribology are pinpointed into Fig. 4.7.1.

- **Insights in nanojoining novel designs**

Established joining processes need to be adjusted and novel joining processes need to be developed for nanoscale joining technologies; a simple extrapolation of macro- to nanojoining techniques is not possible.

Synchrotron radiation and neutrons, in-situ experiments, are unique in allowing a non-destructive analysis and evolution of phases, of the nanostructure and of strain developments during the joining process. This monitoring – with both spatial and time resolution – promises to open up new possibilities for optimising joint micro/nanostructures. This will reveal new joining techniques and will lead to a better understanding of failures in joint structures.

In-situ tests of the joints under loading will provide information about the correlation between the nanostructure and physical and mechanical properties of the joints. In addition, it will clarify our understanding of processes which take place in the bulk material.

Synchrotron radiation topography and diffraction will play a vital role in the elucidation of failure mechanisms and failure progress in welded structures and in in service operation.

Microstructure and properties of dissimilar welds: synchrotron radiation and neutrons are ideal probes for studying phase evolution and strain developments and optimising filler materials and processes.

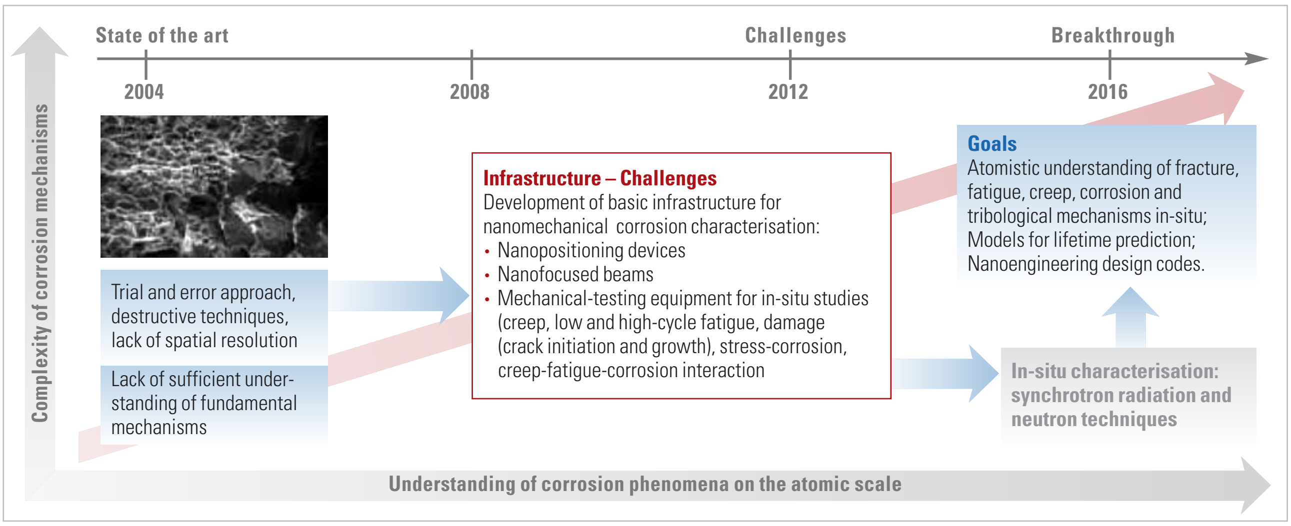

Fig. 4.7.1: Research directions for nanomechanical engineering and design.

Synchrotron radiation and neutron studies form the basis for the formulation of design criteria and codes of practice for nanojoints and nanojoining techniques. An overview of the research directions is given in Fig. 4.7.2.

- **Recommendations**

1. Develop a basic infrastructure for nanomechanical testing at large-scale facilities.
   Engineering nanomaterials properties are of the utmost importance in all nanomaterials designs in various technologies i.e. energy, transport. The relationship between the choice of processing and processing conditions with the resulting nanomaterials and their properties needs to be understood from a scientific point of view but also from an engineering point of view in order to provide high throughput and cost-efficient fabrication processes. Synchrotron radiation and neutrons play key roles in the development of this type of science and engineering and it is essential to develop a modern infrastructure at the large test facilities: beam facilities/availabilities and nanomechanical test equipment adapted for in-situ investigations during the fabrication and accelerated testing conditions. The latter is of particular importance in providing safe and reliable systems and components made from nanomaterials.

2. Create a scientists-engineers/industries European platform.
   An initiative has to be taken to promote this engineering research field in Europe. A GENNESYS Technology Centre would be an ideal catalyst for such an undertaking, to be complemented with European research and development programmes.
   The European nanoengineering programme at large test facilities should have the following mandates:

- To guide the engineers into the new thinking and methodologies of small length- and timescales;
- To reach breakthroughs in nanomechanical engineering, with special emphasis on in-situ testing;
- To characterise the engineering properties under mechanical stress, corrosion/erosion and other simulating industrial environments;
- To promote research and development in nanojoining and tribology (wear, adhesion, friction).

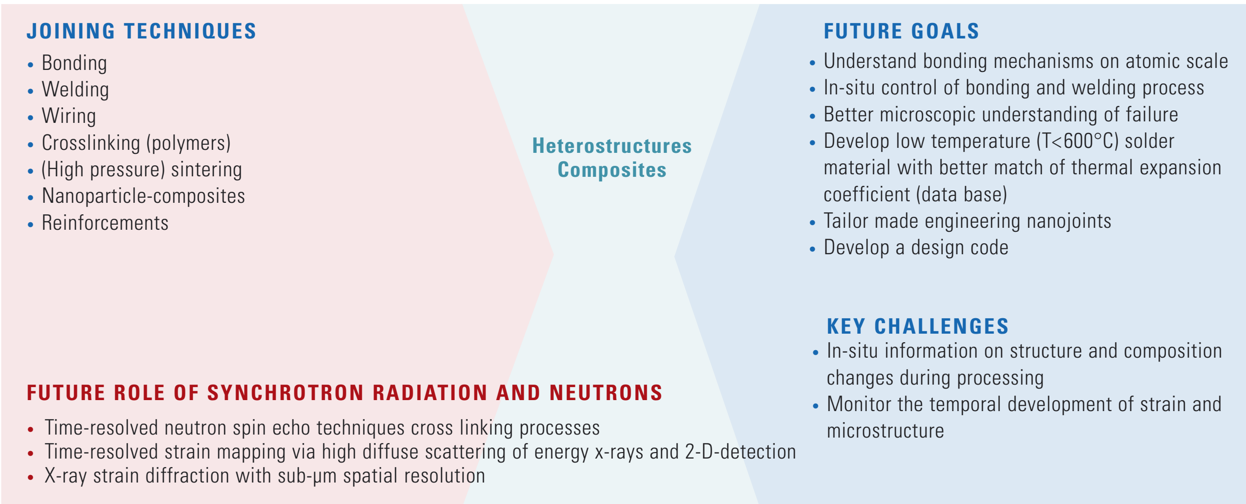

Fig. 4.7.2: Targets and challenges for research on nanojoining techniques.

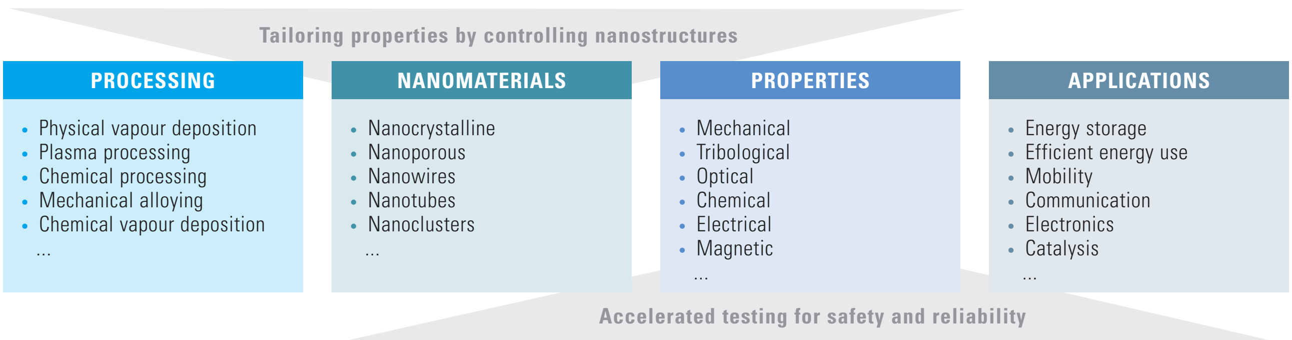

Fig. 4.7.3: Overview of nanostructure fabrication and the need for accelerated testing.

5. SPECIFIC CHALLENGES IN NANOMATERIALS TECHNOLOGIES

5.1. OVERVIEW

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An overview is given in Fig. 5.1.1 of the many domains where nanomaterials will play a key role in technology. It is expected that nanomaterials will fundamentally change products and how they are produced over the next two to three decades.

- Electronics and communications: bio-nanodevices, neuromorphic engineering in transmitting signals directly from the human organism to a machine, quantum computing, recording using nanolayers and dots, wireless technology, molecular electronics, etc. New devices across the entire range of communication and information technologies will be developed with factors of thousands to millions improvement in both data storage capacity and processing speeds, with reduced costs and improved power efficiency compared to present electronic circuits.

- Healthcare and life sciences: nanostructured drugs and delivery systems targeted to specific sites in the body, biocompaticable replacements for body parts i.e. biocompatible coatings for implants and nanopolymers for catheters, sensors for lab-on-a-chip, material for bone and tissue regeneration etc. Medical and life science applications may become the most popular and profitable markets for nanotechnology i.e. cancer research diagnostics and treatment. Nanoscale devices can interact with biomolecules and have the potential to detect disease and deliver new ways of treatment.

- Chemicals and materials: catalysts to improve the energy efficiency of chemical plants, to reduce the exhaust gases of motor vehicles thus lowering the pollution emissions, cutting tools, deep drilling nanomaterials/coatings for petroleum exploration, lubricants, smart textiles.

- Energy nanotechnologies: solar power, clean fossil fuels, new generation nuclear reactors and fusion reactors, new types of batteries, artificial photosynthesis for clean energy, production and storage of hydrogen, energy saving from using lighter materials.

- Food and agriculture: nanoscale pesticides, targeted nanofoods with greater capability and sustainability, nanoseeds, nanopackaging materials.

- Transport: light-weight vehicles.

- Processing and manufacturing: tools to manipulate matter at the atomic scale, sintering of nanopowders into bulk materials with specific properties that may include smart sensors to detect failures and actuators to repair the problems.

- Environment: selective membranes and filters that can remove contaminants, clean water, pollutants from industrial effluents, detection of nanoparticles in the environment, reduced sources of pollution, increased opportunities for recycling.

- Security: detectors of chemical and biological agents, camouflage materials, light and self-repairing textiles, miniaturised surveillance systems.

This chapter highlights the potentials of nanomaterials in various technologies for the next decade and pinpoints the challenges for research and development with special emphasis to the role of synchrotron radiation and neutrons.

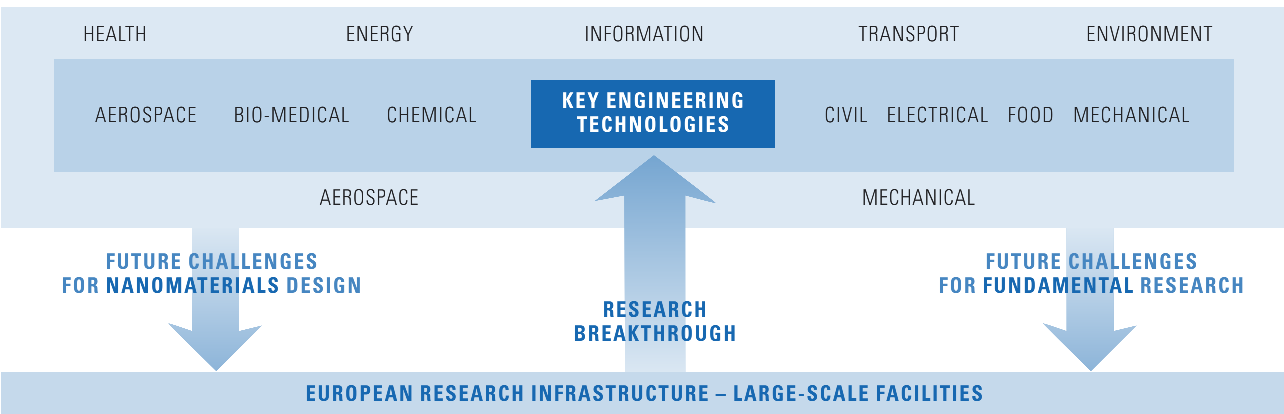
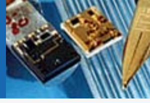


Fig. 5.1.1: Overview of the nanotechnologies.



5.2. INFORMATION AND COMMUNICATION: NANOELECTRONICS AND PHOTONICS

AUTHORS: G. Bauer, G.I. Meijer, J. Stangl, C. Wyon, Y. Bruynseraede, A.V. Chadwick, K.J. Ebeling, W. Eberhardt, L. Malier, K.H. Ploog, P.F. Seidler, A. Trampert, M.H. Van de Voorde

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The future prosperity of information technology strongly depends on further successful scaling processes, creating new devices with higher functionalities, larger flexibility and reliability, all factors, which are prerequisites for increasing the performance of device components. Nanoscience and technology will provide important basic approaches for improved functionalities and new device concepts.

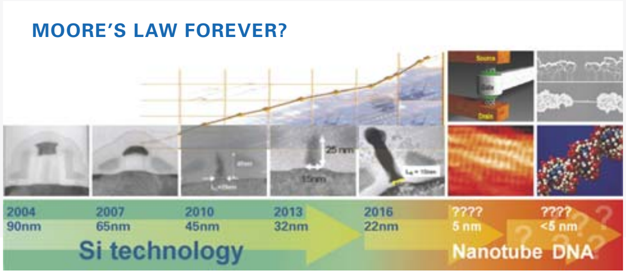

Fig. 5.2.1: Roadmap mapping the future production of increasingly smaller length scales Si-transistors.

CMOS technology

The large interest in advanced materials for electronic and photonic applications is fueled by the reduction trend of the characteristic length scales of electronic devices. Following Moore's law, whereby the number of transistors per squared centimetre of Silicon (Si) would double every 18 months, it is assumed that the characteristic length scales will reach the nanometre size regime in the next years (see Fig. 5.2.1). At the industrial level, this will lead to a minimum feature size of around 10 nm in about 10 years, corresponding to the technology node of 22 nm. However, the laws of physics will ultimately curtail the scaling of conventional complementary-metal-oxide-semiconductor (CMOS) technology.

Identification, selection and implementation of advanced, beyond CMOS technology

Within the semiconductor industry, there is a general consensus that the nanotechnology era, the so-called "beyond-CMOS era", will begin when the scaling capabilities of CMOS technology will have been reached by the year 2020. This nanotechnology era will require new materials, new device structures, and new manufacturing methods. With a commitment by industry and academia to basic research, fundamentally new nanoelectronic approaches to information processing could be explored to sustain the increase of functionality in semiconductor devices.

In its roadmap, the *ITRS 2005*, the Semiconductor Industry Association provides an industry perspective on emerging devices and provides guidance on research needs (see Fig. 5.2.2). The roadmap exhibits diversity in terms of beyond-CMOS nanoelectronic logic and memory devices. Logic devices range from extensions of CMOS using non-planar transistor designs and new materials to fundamentally different approaches i.e. one-dimensional structures containing carbon nanotubes or semiconductor nanowires as critical elements, molecular electronic devices, and spin-based devices. Attractive new memory technologies include magnetic random access memory, ferroelectric memory, nano-floating-gate devices, and phase-change chalcogenide memory.

Parallel progress is made in the fields of photonic bandgap devices, optoelectronic devices, and micro-, and nanoelectromechanical systems (MEMS and NEMS). All these fields of research and development have benefited significantly from the advances in CMOS fabrication techniques.

Future impact of nanotechnology

Hence, nanotechnology will be one of the leading fields of research and development in the century ahead. It will have a variety of applications in practically all domains. It will involve disciplines like electronics, physics, chemistry, and biology, medicine and biotechnology. This joint effort will lead to new device concepts with significantly improved functionalities, possibly as far-reaching as quantum computers and nanorobotics. The impact of nanotechnology will be guaranteed in nearly all social and economic fields.

5.2.1. NEW NANOMATERIALS FOR NEW ELECTRONICS

The ITRS roadmap predicts the main trends in the semiconductor industry, identifies the technological barriers and provides an industry perspective on current and emerging devices. The following section will address selected challenges to extend the integrated circuit technology to, and beyond the end of CMOS scaling.

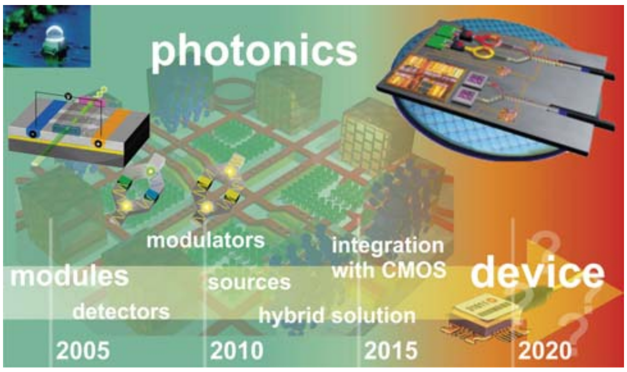

Fig. 5.2.2: The Semiconductor Association provides in its roadmap, the *ITRS 2005*, an industry perspective on emerging devices and provides guidance on research needs.

New gate oxide materials

The performance of microprocessors is enabled primarily by the length of the transistor gate. The continued reduction of the gate length accompanies an approximately proportional reduction of the gate oxide thickness. In 2007 a gate oxide thickness of 1 nm was reached. The tunnelling of leakage currents is becoming predominant. High-dielectric-constant gate oxides have to be used to suppress the tunneling current while maintaining the drain current. In addition, metal gates with appropriate work functions have to be introduced to minimise the depletion width in the gate electrode. It is most likely that strained Si channels will be utilised to enhance carrier mobility. All these material changes pose a great challenge in CMOS technology, where SiO_2/poly Si has long played a central role as the most reliable gate stack system.

DRAM technology

DRAM technology focuses on the construction of memory cells with ever smaller areas. This pressure to minimise the cell size is, however, in conflict with the requirement to maintain a certain memory capacitance to ensure reliability of stored data. Therefore, creative approaches in terms of design and materials are required to meet the minimum capacitance requirements while reducing cell size. Currently, higher-dielectric-constant materials along with a 3-D memory structure are envisioned.

System-on-chip

Significant effort is placed on integrating different emerging technologies on conventional Si-CMOS, so-called "system-on-chip". It is foreseen that, for cost-related reasons, Si will remain the integration platform. One field of research and development will address optical interconnects. While for long-distance communication optical transmission has replaced electric wiring already, photonics will have to accomplish this for high-speed data transfer over shorter distances. Already, processing power has shifted to external components like graphics adapters and bus controllers. This creates a demand for fast data links between those processors and controllers. Roadmaps for the according photonics development, for instance the development of couplers and transceivers between optical lines and semiconductor chips, required for the transition from electronics to photonics, are currently established. While basic research is conducted on different solutions based on Si, III-V semiconductors, and organic materials, current industrial research focuses on Si-based solutions.

Bottom-up approaches and self-assembly

The fabrication technologies applied so far in industry may be subsumed under the term "top-down approach", where lithographic patterning of larger structures creates small structures. In research, different strategies have been developed that may be subsumed as the "bottom-up approach": nanostructures are composed of small units (atoms, molecules). Self-assembly is very promising for the hierarchical organisation of nanostructures, a concept that imitates processes in nature. In the mid-term perspective, a combination of "top-down" and "bottom-up" approaches is likely to be used. Self-assembled nanostructures are used in certain device areas, for example, magnetic memories based on quantum dots. Possibly, a single-electron transistor could be realised using quantum dots, in order to make an electrical switch with the charge of a single electron.

Carbon nanotubes

Carbon nanotubes can be used either as semi-conductors or as metals. Potentially, carbon nanotube devices, resembling a one-dimensional quantum-mechanical system, could provide a gain in clock frequency and lower power consumption. Major challenges for nanotubes are their controlled fabrication (monodispersity), contacting to electrodes and the controlled positioning required for integration (see Fig. 5.2.3). Semiconductor nanowires are currently being developed. The principle functionality as transistor has already been demonstrated. Provided their integration into devices at an economically relevant level is developed, they might be used beyond the 10 nm technology node. The advantage of semiconducting nanowires is that they can be produced with control over length, diameter, and position on a substrate. Issues such as doping and contacting have to be addressed to make nanowires usable for integrated devices, but this seems to be easier to accomplish in the mid-term perspective than for carbon nanotubes. Whether or not graphene-based electronics will appear within the next 15 to 20 years remains to be seen, despite the huge amount of basic research devoted to this subject.

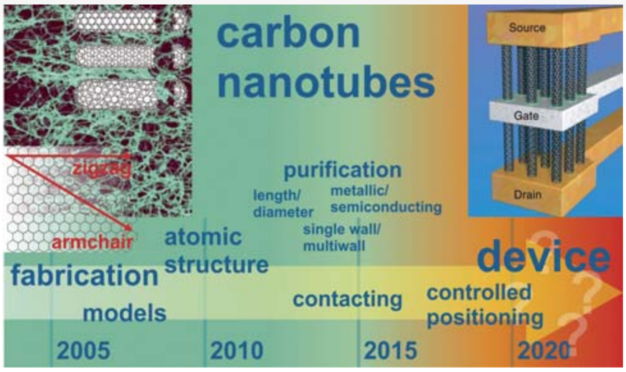

Fig. 5.2.3: Roadmap presenting challenges for nanotubes research.

Spintronics

Spintronics utilises the spin of electrons for advanced devices and novel device concepts. Currently this technology can be found in all state-of-the-art read-heads of hard disk drives. Furthermore, magnetic random access memory (MRAM), based on magnetic tunneling junctions, is about to be introduced on the market. MRAM has the advantage of being non-volatile and it offers the potential of a larger storage density than DRAM since no capacitor is required. Fundamentally different device concepts such as spin-transistors are in the basic research phase (see Fig. 5.2.4).

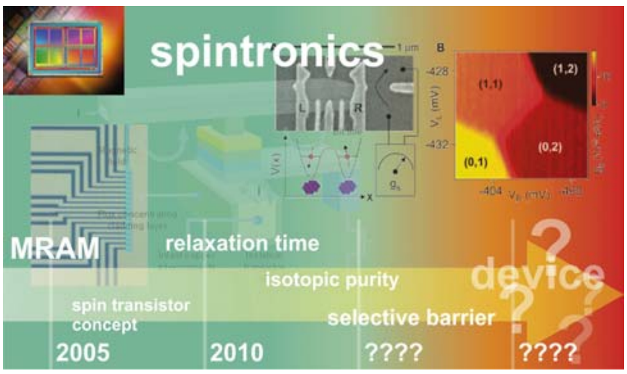

Fig. 5.2.4: Roadmap presenting the major challenges for spintronic research.

Developing new post-CMOS device concepts that enable further performance increase and cost reduction requires:

- Experimental materials research, including facilities for the fabrication of novel device concepts and advanced functional materials; metrology to characterise their critical properties;
- Modelling and numerical simulation to effectively predict the functionality and physical properties of emerging devices and novel materials, respectively, and gain full understanding of the underlying mechanisms;
- Research laboratories of the semiconductor industry are considering several concepts beyond charge-based information processing for the period after 2015–2020. Intensified research is mandatory to be able to identify the concepts which will lead to viable technological implementations. As "lab-to-fab" development takes 10 to 15 years, research efforts are needed now;
- A network to effectively link the efforts and results of individual institutions;
- A large number of well-trained scientists and engineers.

5.2.2. CONCLUSIONS AND RECOMMENDATIONS

Future role of synchrotron radiation and neutron facilities

Synchrotron radiation and neutron technologies have played an important role in materials research and nanotechnology for advanced materials characterisation to help determine whether novel materials have the necessary performance characteristics for device applications (see Fig. 5.2.5. and 5.2.7). In particular:

- The formation and evolution of point defects and stacking faults in semiconductors occurring during dopant implantation and subsequent annealing (x-ray and neutron diffraction).
- The properties of dislocation networks (x-ray topography). Using synchrotron radiation, x-ray topography and diffraction were combined.
- Imaging of the strain fields around defects and in devices (x-ray topography and diffraction).
- Minute contamination concentrations (x-ray fluorescence).
- Precise quantitative (standardised) measurement of magnetic moments (neutron metrology).
- Hydrogen monitoring (neutron technologies).
- The roughness and interdiffusion of interfaces in e.g. semiconductor laser devices (x-ray/neutron reflectivity).
- The chemical composition distribution and strain profile in nanostructures (glancing angle diffraction technologies).
- Monitoring of the composition and strain profiles in SiGe devices (glancing angle diffraction technologies).

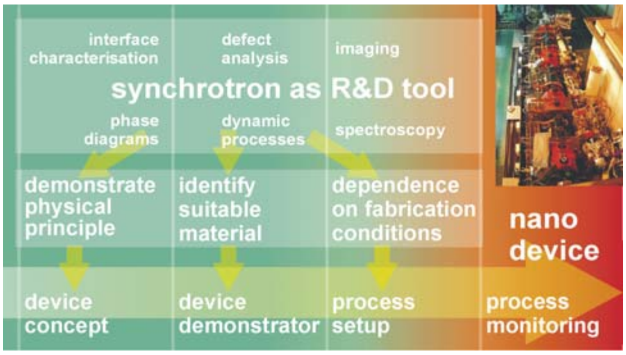

Fig. 5.2.5: The synchrotron R&D tool.

In the future, the importance of synchrotron radiation will increase strongly. The success of the nanoelectronics era will critically depend on finding alternative materials and on the introduction of new types of logic and memory concepts. This grand challenge will require metrology for a non-destructive characterisation of critical materials properties at the nanometre scale. Synchrotron radiation and neutron techniques will play a significant role in this major materials research effort. With decreasing device size, the volume available for characterisation is significantly reduced and, the ratio of surface (interface) to volume is dramatically increased. Consequently, the study of interfaces and surfaces will be of the utmost importance. Synchrotron radiation has been established as one of the most important tools for this purpose.

Future urgent needs include:

X-ray nanoprobe technology

Synchrotron radiation with high spatial resolution ("x-ray nanoprobe") is urgently needed to characterise, at device scale, the various properties of magnetic materials envisioned for:

- Spin devices;
- High-dielectric-constant materials for logic and memory;
- Low-dimensional semiconductors.

Precise and reproducible sample positioning systems are required. The x-ray nanoprobe should provide for spectroscopy, diffraction and transmission imaging. The combination of several modes (diffraction, transmission imaging, fluorescence, spectroscopy, and magnetic diffraction) in a single experimental tool will produce unique characterisation capabilities for the nanoscience on photonic and electronic nanostructured materials. It must be clarified whether brighter x-ray sources are required in the near future (Energy Recovery LINACS) because the efficiency of focusing elements is physically limited.

In-situ characterisation capabilities

- Reliable diffraction techniques are needed to provide information on structural properties (transition temperatures, interface stability, reversibility and stability of phase changes).
- Spectroscopy techniques are needed to study the electronic properties (density of states, work functions, and possibly charge trapping).
- Diffraction combined with spectroscopy has to be further developed for the characterisation of magnetic properties (transition temperature, spin relaxation, interface spin transmission, and spin decoherence).

X-ray source and beam line developments

- Considerable developments of undulator-based x-ray sources and beam line equipment are required. Existing sources should be refurbished based on these developments. In addition, other concepts (energy recovery after one round of an electron bunch) will be required in order to meet the research demands in the coming decades. To this end, new synchrotron radiation centres have to be built; their design needs to be worked out within the next 5 years, so that they can become operational within about 10–15 years. In parallel, further capacity for wider industrial use of synchrotron sources has to be created, as detailed in Fig. 5.2.6.
- Improved x-ray detectors with higher sensitivity and dynamic range and position resolution are needed.
- The analytical potential of future free electron lasers (FELs) for the semiconductor technology must be investigated in detail.

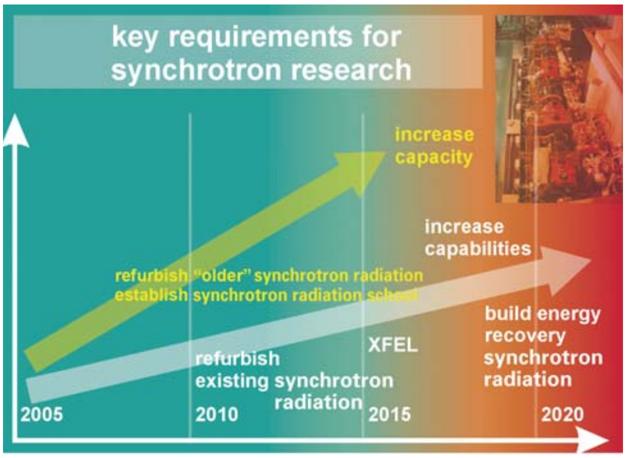

Fig. 5.2.6: Key requirements for synchrotron research.

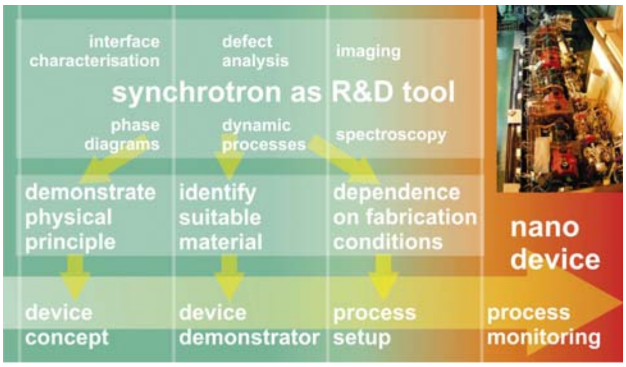

Fig. 5.2.7: Key contributions of synchrotron research.

The following semiconductor innovation areas require a strong involvement of the synchrotron radiation and neutron facilities:

- Si (Nano-)electronics: functional materials compatible with silicon;
- Spin- and magneto-electronics: ferromagnet-semiconductor hybrid structures;
- Optical communication network and systems: photonic-bandgap materials, single photon sources;
- Organic LED's, displays, sensors, electronics: organic materials with high thermal stability, low power consumption;
- Solid state lighting: epitaxial and bulk growth; materials including nanomaterials and substrates; phosphors;
- Solar cells, UV-detectors, sensors and actuators.

Nanomaterials characterisation is of the utmost importance, synchrotron analysis is one very important tool for this purpose (see Fig. 5.2.8); The same characterisation tools will be applied to all of the above mentioned research fields. Urgent actions to be undertaken in the near future:

- The number of beam lines capable of nanoprobe analysis has to be increased;
- Beam lines offering the combination of diffraction, imaging, and spectroscopy need to be established;
- Complementary analysis technique has to be established on site or in close proximity;
- Advanced magnetic scattering and spectroscopy stations at synchrotrons and neutron sources have to be established;
- The capacity of in-situ and in-vivo experimental stations has to be increased;
- A critical mass of scientists and engineers has to collaborate. Information flow and knowledge on techniques and capabilities of facilities is essential.

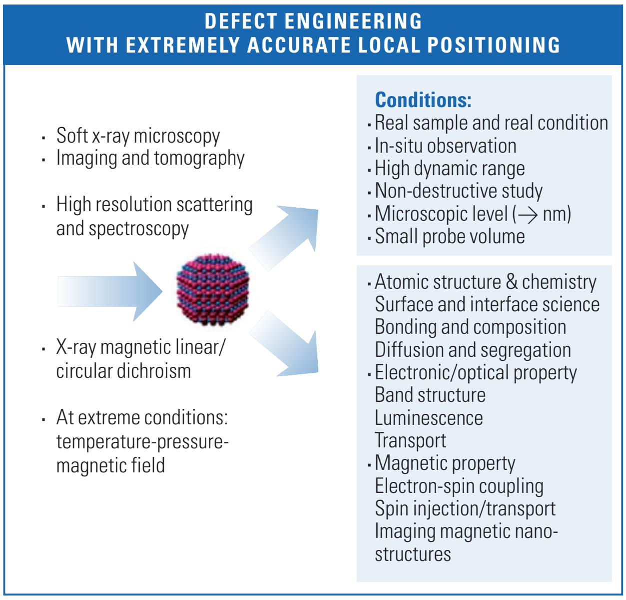

Fig. 5.2.8: Defect engineering with extremely accurate local positioning.

Synchrotrons and industrial use of synchrotron radiation: policy requirements

If industrial processes are developed or if standards for process control have to be determined, typically a systematic series of essentially identical characterisation measurements is required. At present, this mode of operation is difficult to implement in current synchrotron radiation and neutron facilities.

Nevertheless, industry recognises the potential that is offered by the use of synchrotron radiation and neutron facilities for the development of new products. At synchrotron radiation sources, in the period from 2000 to 2005, the beam time sold to industry for proprietary research and development has increased by a factor of 5, and corresponds now to about 5% of the total allocated beamtime.

In order to attract future additional industrial work at synchrotrons, the following measures should be considered:

- Extension of the infrastructure to meet the needs of industry. Next to providing access to state-of-the-art synchrotrons, provide additional capacity by refurbishing second generation synchrotron sources. In order to keep the research in Europe competitive, additional funds will be needed.
- Attract new users from industry. The most efficient way will be to educate master and PhD students at synchrotron radiation and neutron facilities, who subsequently bring their knowledge into industry and will advocate synchrotron- and neutron experiments.
- Transfer of new developed x-ray metrology to industry: industry is sometimes unaware of recent progress in x-ray methods. An institution promoting the knowledge transfer and collaboration between industry and synchrotron radiation/neutron researchers is needed;
- Create a European centre of technology which serves as stimulus and coordinator and protector of the rights for industry to the large test facilities.

GENNESYS European Technology Centre "Electronic and photonic nanomaterials "

The development of novel functional nanostructured materials will demand an industry-guided European Technology Centre located at and closely linked to a synchrotron radiation/neutron facility. The task of this new centre will be:

Precision characterisation of the physical basis of the functionality

This includes:

- A fundamental understanding of the electronic and photonic interaction in nanostructured materials;
- A precise control of the material properties at the level of the electron and photon wavelength;
- A systematic and atomistic understanding of the role of interface structures.

Advanced materials search and development

The development of new materials beyond silicon and combinations with silicon will be inevitable.

Advanced analytic technologies in urgent/emerging material problems (see Fig. 5.2.9).

- Si (Nano-)electronics: high-k materials compatible with silicon;
- Spin- and magneto-electronics: ferromagnetic-semiconductor hybrid structures;

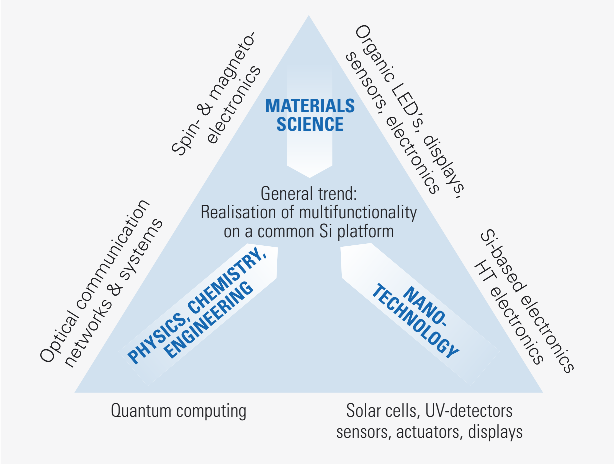

Fig. 5.2.9: Potential areas for functional nanomaterials in electronics/photonics.

- Organic LED's, displays, sensors, electronics: organic materials with high thermal stability, low power consumption;
- Solid state lighting: epitaxial and bulk growth; materials including nanomaterials and substrates, phosphors;
- Optical communication network and systems: photonic-bandgap materials, single photon sources;
- Solar cells, UV-detectors, sensors and actuators.

A successful research and development of future functional nanostructured materials for electronics/photonics requires the combination of competences from different scientific and technological areas: materials growth – nanotechnology – nanoanalytics – physics/chemistry/engineering/biology. This challenge justifies the installation of a European Technology Centre "Electronic and Photonic Nanomaterials", which must incorporate the following capabilities (see Fig. 5.2.10 and 5.2.11):

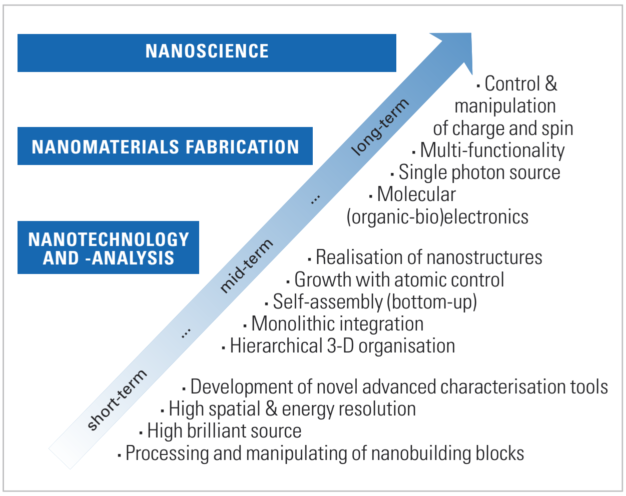

Fig. 5.2.10: Research and development of nanostructured materials for electronics and photonics.

Nanomaterials fabrication

- Growth of artificial nanostructures with atomic precision;
- Self-assembly on crystalline substrates with well-defined interfaces;
- Ability for monolithic integration.

Nanoscience

- Basic understanding of the physical and chemical properties determining the functionality of the nanomaterials;
- Development of new concepts and strategies for multi-functional devices with higher performances.

Nanotechnology

- Processing of isolated, free-standing three-dimensionally arranged nanostructures;
- Controlling and manipulation of single nanobuilding blocks for 3-D arrangements.

Advanced online characterisation technologies

- Monitoring the structural, electronic and photonic phenomena with atomic-scale spatial resolution;
- Defect engineering;
- Nanobeam capabilities;
- In-situ studies (long-time): function-performance-degradation-failure.

Nanomaterials modelling

- Multi-scale modelling capabilities of electronic, photonic and magnetic functions.

The formation of a European Competence Cluster located at a synchrotron radiation/neutron facility operating with thematically linked laboratories throughout Europe via modern information technologies (internet, video conference, remote control experiments). The operation scheme must have a high level of flexibility to respond to new trends and research topics, and must be receptive to external cooperation with industrial partners. This is needed to be able to keep up with the very short development cycles for every next product generation.

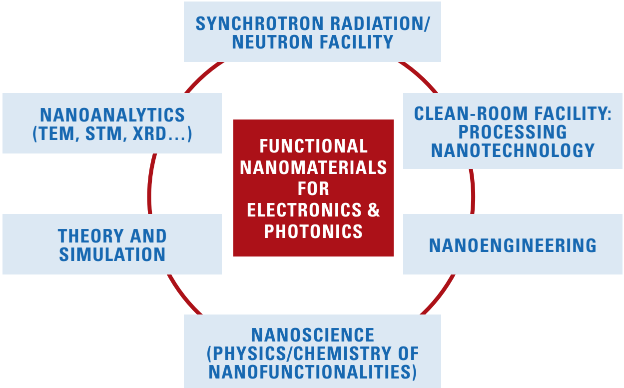

Fig. 5.2.11: Competence cluster for research and development of novel functional materials for electronics and photonics.

5.3. BIO-NANOSYSTEMS

AUTHORS: A. Bravin, R. Borsali, J.A. Bouwstra, A. Buleon, B. Cathala, A. Cesàro, P. Couvreur, K. de Kruif, J.K.G. Dhont, A.M. Donald, J. Doucet, P. Fratzl, G. Gompper, V. Guyot-Ferreol, I.W. Hamley, R.A.L. Jones, K. Kostarelos, E. Perrier, M.L. Saboungi, R. Sammons, H. Schenk, P. Schurtenberger, P. Vadgama, D.J. Wood

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5.3.1. OVERVIEW: BIO-NANOMATERIALS TECHNOLOGY

The scale-length reduction now achieved through the adaptation of a new armoury of nanosynthetic and nanomachining technologies has the potential to interact with the biological matrix in an unprecedented manner. Biological systems in general, and the biological response in specific in the context of biomaterials implants – whether in tissue or in blood – is able to recognise nanoscale architectures. It is thus now timely that nanoforming technologies are fully harnessed in order to manipulate the nature of the implant-biomatrix interface and thereby enhance implant performance and clinical efficacy.

Key challenges and research needs (Fig. 5.3.1 and Fig. 5.3.2)

- There are considerable challenges in the design of nanostructures which can operate reliably over extended timescales in the body. Indeed, for each new nanomaterial design, it has become mandatory to consider toxic and other undesired effects, irrespective of any enhanced functionality. Nanostructures embedded in an organised matrix such as a nanocomposite have demonstrated improved mechanical properties. They also have the potential to mimic some of the complex biomechanical properties of hard tissues, and perhaps structurally important soft tissues such as blood vessels. However, it is as surface structures that organised nanomotifs can especially help to direct organised cellular response, modify flow phenomena, control the nature and extent of protein deposition and in doing so, condition long-term dynamic processes that define the timescale for good biomaterial performance. Both surface chemistry advances and new film deposition capabilities will augment these key-functions, allowing for greater interfacial control and molecular fine-tuning.
- Reproducible design and forming technologies need to be developed specifically for biomaterials for application in the full range of current materials sources – ceramics, metals, polymers. Each have different forming requirements and, once formed, have a level of surface reactivity that may be qualitatively different to macroscale counterparts. This is especially true for the reactivity in the body. The twin processes of encapsulation and corrosion therefore could be amplified with high surface area structures. Polymeric surfaces decorated with active biomolecules may lead to greater bioactivity to influence these processes in biological tissues. The fundamentals of these processes are less well understood and there is a major need to investigate these, preferably using non-destructive and non-contact techniques.
- At the nanoscale, molecular and structural domains converge and it is likely that a multiplicity of surface properties and surface cues impinge upon the "reaction coordinates" of the biological response. The challenge is to observe these effects at the nanoscale. For this, greater levels of length, time and concentration resolution are demanded than have been achieved so far. Without this, mainly end-stage outcomes will be characterised without the all-important initiation stages being detected. The right combination of biomimetic structures could allow for reactive, and thereby intelligent, biomaterials. With incorporated nanoelectronic communication components, remote interrogation should also be possible.
- Forming techniques require considerable refinement to produce predictable structures and to assemble them at surfaces in a tailored manner for specific functions. It is likely that future hybrid

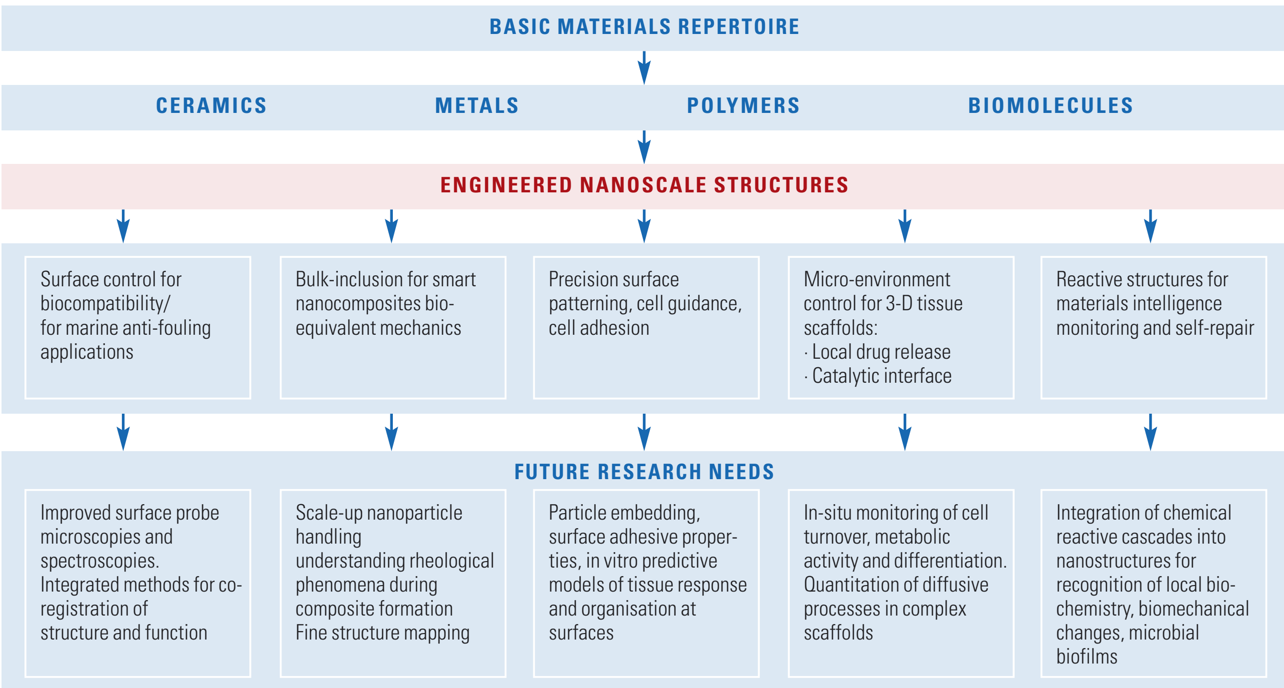


Fig. 5.3.1: Nanoengineering strategies and underpinning research topics for practical applications.

structures will be developed incorporating, say, a combination of polymers and ceramics or involve the integration of natural biomolecules and synthetic materials. While this may allow for better replacement of physiological function, the synthetic challenges are substantial – all would benefit hugely from improved monitoring technologies. Advanced forming techniques will underpin drug delivery, giving unprecedented control over the timing, location and release dynamics of potent, therapeutic agents.

- The response of surface active colloids, notably proteins, (and cells), to a surface brings about major structural and orientational changes and they have yet to be mapped in any systematic way. Protein remodelling, denaturation and exchange (lateral, vertical) at surfaces is conditioned by material surface properties, but as yet, predictive modelling has been elusive.

- Aside from the biomedical field, nanomaterials will play a fundamental role in new environmentally benign coatings to preventing marine fouling. Engineering and manufacture of nanostructured anti-fouling coatings for ships and water purification facilities need to be improved in order to become sufficiently economically feasible.

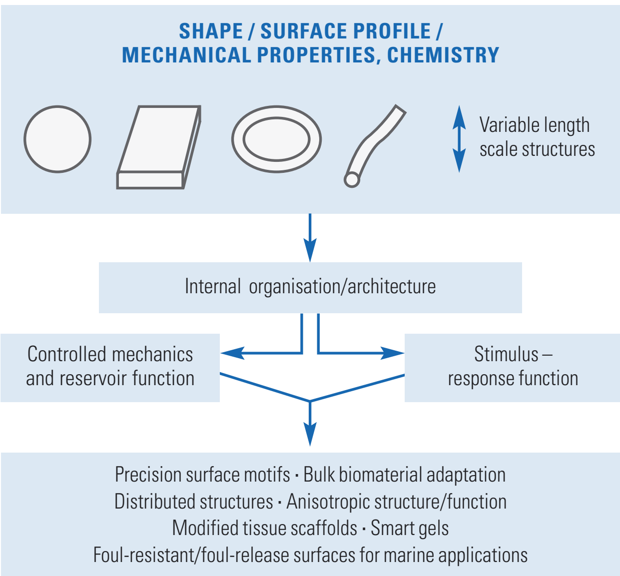


Fig. 5.3.2: Basic design features of individual nanostructures and their functional outcomes.

Future role of synchrotron radiation and neutron facilities

(Fig. 5.3.3)

- The high spectral and spatial resolution in diffraction, spectroscopy, imaging and microscopy which has become available at modern synchrotron radiation and neutron facilities opens up entirely new ways of monitoring dynamic nanoscale phenomena.
- Neutrons are particularly useful to detect the hydrogen in biological systems which enable particularly useful information during atomic scale structural changes, as during protein folding. The role of water at and near surfaces in macromolecular hydration and dynamic exchange must be explored using combined x-ray and neutron analysis.
- It should be further explored how synchrotron radiation could be employed both for nanopattern formation and modification.
- Interface-sensitive diffraction and spectroscopy techniques have to be exploited in order to analyse in-situ the role of the Helmholtz double layer and hydration effects on disagregation, denaturation and remodelling of natural macromolecules.
- X-ray microscopy must be further optimised in order to allow damage-free operation in biological environments, allowing, monitoring of environmental effects on the structure during extreme changes associated with the tissue response to a biomaterial surface.
- Ultrafast dynamic diffraction and spectroscopy of the cell membrane-surface interaction and correlation with surface nanodomain properties must be developed to a reliable standard to help understand adhesion phenomena in relation to surface chemistry.
- Various complementary analytical (particularly spectro-imaging) techniques should be implemented in future synchrotron radiation beam lines to monitor the cell organelle and cytoskeleton and their external contacts to nanostructures, allowing establishment of precise cell triggers which influence and control cell attachment at (nanostructured) surfaces.
- All available synchrotron radiation and neutron techniques should be exploited to establish a solid database of polymer bulk and surface properties within tissue scaffolds for tailoring the scaffold design by a 'bottom-up' approach.
- Dedicated synchrotron radiation and neutron beam lines for non-destructive in-situ analysis of biological systems would underpin the entire biological programme. Surface modification and creation of nanoarchitectures should be an integral part of future research activities. These efforts should be complemented by a clear materials metrology programme. Crucial to a successful research strategy are on-site facilities for cell culture, cell and protein separation and characterisation, including available biological models for the study of surface biocompatibility.

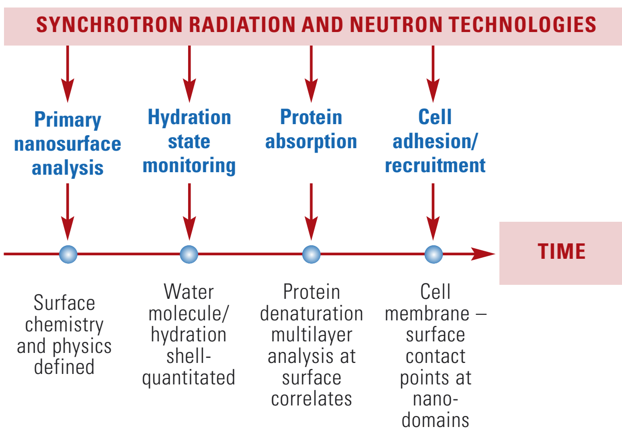


Fig. 5.3.3: Application of synchrotron radiation and neutron scattering along time-dependent events during nanomaterial contact with a biological matrix.

5.3.2. MATERIALS AND TECHNOLOGY IN MEDICAL SCIENCE

Biological systems are organised into nanostructural unit components which then combine to form the well-known macrostructures as observed by conventional microscopes. This is readily understood for membrane bound cellular organelles such as mitochondria, the Golgi apparatus and secretory granules. However, less accessible nanostructures such as enzyme complexes and connective tissue sub-elements are also highly organised at the nanoscale. Interaction of nanomaterials with natural biological systems therefore, clearly, not only has a direct impact on the operation of nanostructures, but a dynamic end outcome that may be quite different from that assumed on the basis of conventional soluble agents.

Nanomaterials as either solid or hollow structures offer the opportunity of "stealth" delivery of a materials component or a chemical payload to a specific, designated tissue and cellular scale. Embodied in this is a universal concept of nanomaterials, which provides highly specialised, independent functions within one structure. These are: penetration of natural whole body and tissue barriers, selective tissue targeting, quantised delivery of a chemical payload. The designed payload may be therapeutic, e.g. for cancer or gene therapy for distributed monitoring as a basis for understanding the operation of natural nanostructures.

Through materials design and new forming methods, it is likely that the desired nanostructures with complex natural systems will be fabricated to play an important part in the diagnostic and therapeutic armoury of the clinician. In-vitro labelled nanoparticles may act as biosensing interfaces with inherent signalling properties that can be scaled up for high throughput screening.

Research needs (Fig. 5.3.4, Fig. 5.3.5, Fig. 5.3.6)

- New modes of nanomaterial synthesis are required which encompass an integrated repertoire of metal, ceramic and (bio-)polymeric forming techniques. These will benefit from an improved understanding of biological self-assembly, the structural organisation of biological (supramolecular) structures, as well as their functional correlates.

- Simultaneously, there is a need to study the behaviour of controlled atomic nanostructure assemblies directly in complex biological fluids at epithelial interfaces and at cell membrane surfaces. In particular, this demands too much closer study of the linkage between the surface physicochemical properties of nanostructures and the influence of this on interactions as with surface active biological macromolecules, cell membranes and intact cells.

- There is a need for the surface texturing and modification of nanoparticles, quite independently of any bulk organisation. This may be achieved by the attachment of controlled monolayers and end-attached polymers at solid nanoparticles or by the formation of hollow nanovesicles independently loaded with required soluble and solid state agents.

The study of supramolecular scale operations as a part of critical biological processes has been limited by conventional techniques. A key structural target that would repay closer analysis is the lipid bilayer membrane which defines the partitioning and phase boundaries between cellular and sub-cellular structures. Not only do cell receptors and channel proteins within these function as nanostructures, but the lipid phases themselves function as a dynamic, combinatorial boundary, continuously recycling – in itself a nanoconstruct.

Artificial nanoparticles need to interact with lipid membranes in order to effect specific cell changes. Accordingly, both a study of the cell membrane and of its binding interactions with the nanomaterial surface are required in order to establish predictive modes for therapeutic delivery.

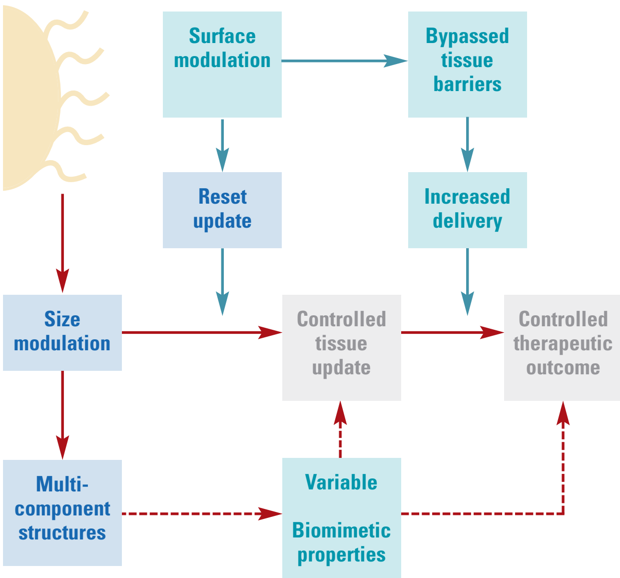


Fig 5.3.4: Surface and scale properties of nanoparticles as starting points for controlled uptake and therapy.

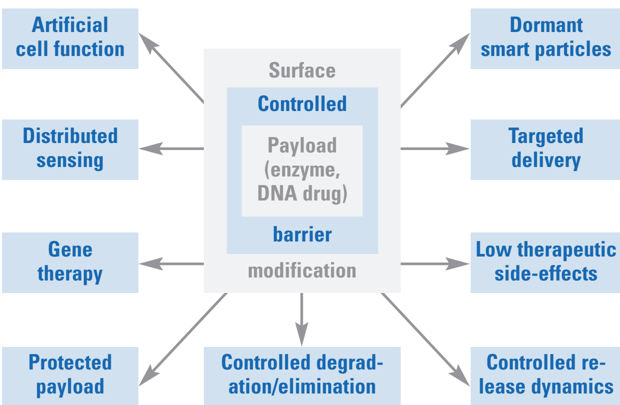


Fig. 5.3.5: Individual sub-elements of a nanostructure and functional outcomes.

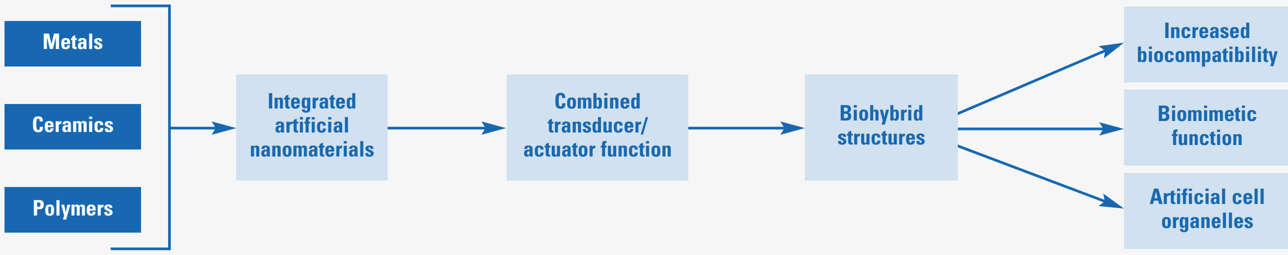


Fig. 5.3.6: Integration of biological components to enhance biological-equivalent functions.

Future role of synchrotron radiation and neutron sources

(Fig. 5.3.7)

- Using modern analytical technology provided by current and future synchrotron radiation and neutron facilities, rapid particle contact-induced change can be followed, linked to the biophysics of interaction. The final goal is that future understanding leads to nanomaterials which could replace or repair defective membrane structures.
- Nanomaterials are inevitably modified by exposure to biological fluids. Specifically, surface interactions with proteins dominate the processes leading to loss of selective targeting and potential redirection of nanoparticles so they become sequestered by different tissues. The nature of the surface biomodification, its continued remodelling and further environmentally sensitive change could be ideally studied at the nanoscale using Synchrotron radiation and neutrons, thereby fostering a better understanding of uptake and dissolution processes.
- The use of complementary monitoring techniques can bring our understanding to a level where nanomaterial design can be advanced sufficiently to enable effective therapeutic and diagnostic use of nanomaterials.
- The use of x-rays and neutrons will be possible to monitor nanoparticles within intact tissues and across blood vessel walls. In addition, the correlation of the tissue microenvironment and its morphology with the passage of such particles to the eventual cell target would help define the polymeric and fluidic tissue barriers to successful delivery.
- Micro-/nanofluidic flows through the extracellular tissue matrix, the capillary network and through specialist tissue channels such as those found in muscle, bone and the lymph (including respiratory channels) are influenced by surface and wall effects; high resolution dynamic techniques are needed not only for analysis of these structures, but to better understand the transport behaviour of nanomaterials within them. There is the potential of stronger links with predictive biological modelling.

Overall conclusions and recommendations

- Develop nanoparticles with modified bulk and surface properties for adaptive transport across in-vivo cellular and acellular barriers.
- Integrate understanding of normal cell membrane structures with contact effects at nanoparticles and the biophysics of particle assimilation.
- Develop nanoparticles and other nanostructures with sensing, actuating, targeting and drug release capabilities, respectively.
- Develop in-vitro tissue models for nanomaterial testing that facilitate application of synchrotron and neutron studies. Monitoring uptake, as well as elimination.
- Apply synchrotron radiation and neutron characterisation techniques to normal and abnormal natural bionanostructures, e.g., prion protein, viral coats, amyloid plaques, atherometous vascular deposits.

High relevance of synchrotron radiation and neutron sources:

- Nanomaterial forming and characterisation facilities, including organic synthetic facilities for derivatisation work;
- Dedicated facilities for biological study;
- On-site tissue culture and biochemistry facilities for preparation of cell; membrane and subcellular model systems;
- Availability of additional analytical facilities for protein and lipid biochemistry, drug analysis, probe microscopy.

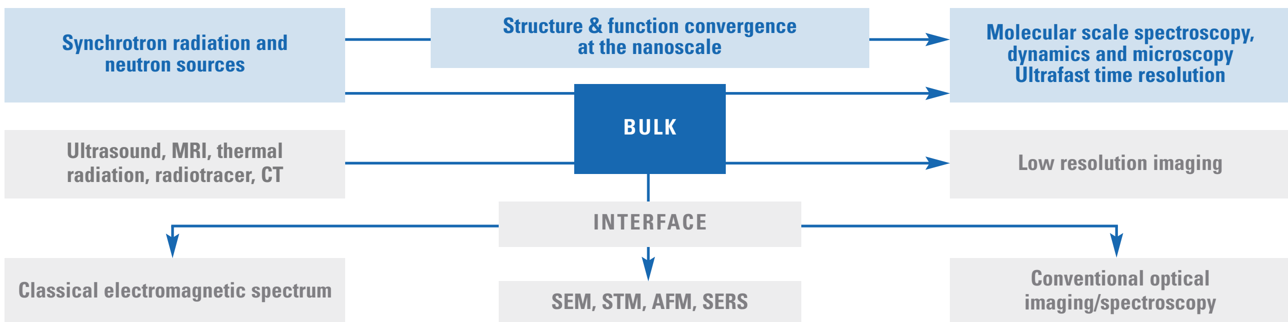


Fig. 5.3.7: Analytical techniques for bulk versus surface characterisation and the relevance of synchrotron and neutron sources for high resolution studies.

5.3.3. MATERIALS AND TECHNOLOGY IN DENTISTRY

Introduction and overview

"Nanodentistry" can be defined as the science and technology of diagnosing, treating and preventing oral and dental disease, relieving pain, and of preserving and improving dental health, using nanoscale-structured materials. Nanotechnology has already started to have an impact in several of the dental specialities including periodontology, implantology, prosthetic dentistry, orthodontics and endodontics. Important areas of dental research involving bio-nanomaterials are shown in Fig. 5.3.8.

Research needs in the future

As medicine advances and people live longer, nanodentistry will play an increasing role in enabling people to keep their natural teeth and oral tissues healthy and functioning for as long as possible. Examples of areas of research which will involve nanotechnology are listed below:

1. Tooth development: Understanding how teeth develop in the embryo will lead to the development of novel biologically based therapies to supersede more traditional approaches for treatment of tooth disease.

2. Tooth structure: Understanding the structure of dentine and enamel and assembly at the molecular level will enable the development of biomimetic methods of repair and regeneration.

3. Reconstruction of hard and soft periodontal tissues:

- Development of new biomimetic resorbable membranes for guided tissue regeneration, promoting formation of new periodontal ligament, bone and soft tissue.
- Development of artificial protein matrices that bind hydroxyapatite, together with growth factors, as bone substitute graft materials that promote stem cell differentiation into osteoblasts.

4. Caries treatment:

- Development of superior composite filling materials for replacement of amalgam for posterior teeth with materials with excellent aesthetics, mechanical properties and longevity.
- Scientists are already experimenting with the use of high-precision powder jet blasting with hydroxyapatite nanoparticles for ablation of carious enamel/dentine and simultaneous formation of an hydroxyapatite-coated bioactive surface.
- Remineralisation: Development of materials to interact with the tooth enamel and dentine for biomimetic remineralisation and repair of damaged teeth.

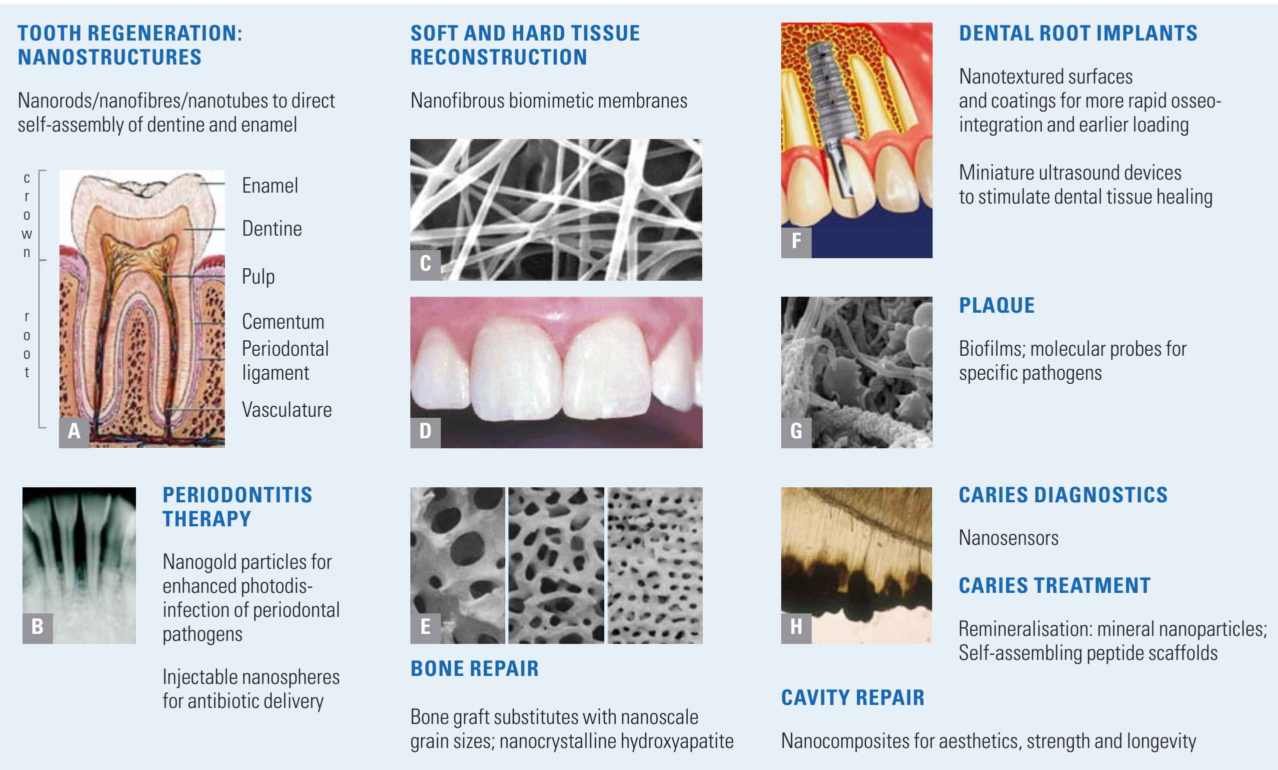


Fig. 5.3.8: Overview of some of the applications of nanotechnology in dentistry. A) Anatomy of the tooth; B) Radiograph showing bone loss in periodontal disease; C) A nanofibrous membrane for soft tissue repair to mimic the natural extracellular matrix; D) Composite fillings must match as closely as possible the colour and translucency of natural teeth; E) Hydroxyapatite scaffolds for bone repair; F) Diagramme (DENTSPLY Friadent), of a dental implant showing osseointegration; G) Scanning electron microscopeimage of dental plaque showing mixed bacterial biofilm and cells. H) Tooth section showing caries developing in the enamel.

5. **Periodontal disease:** Understanding the aetiology and pathogenesis of these diseases, focusing on the molecular and cellular pathways and the interaction between bacterial and patient factors such as bacterial population dynamics, virulence factors and stress hormones, will lead to prevention and novel ways to halt the progression of the disease.

6. **Prosthetic dentistry: Development of dental root implant materials** with superior mechanical properties preventing stress shielding of adjacent bone and with biomimetic surface properties promoting rapid ossification and long-term stability, especially for patients with inferior bone stock and healing properties.

7. **Development of materials for maxillofacial and alveolar bone repair and augmentation** with superior mechanical properties and controllable resorption rates. These totally synthetic artificial nanocomposite materials will replace autologous bone (from the same patient) to avoid the pain, discomfort and risk of infection that is often associated with a bone graft procedure.

8. **Salivary and respiratory diagnostics:**

- The development of molecular probes and sensors for biomolecules within saliva and plaque will facilitate early diagnosis of diseases such as caries and periodontal disease.
- The oral cavity as an easily accessible site where molecules may be detected in our breath, in saliva or oral mucosal tissues that can indicate the presence of systemic disorders and diseases such as cancer. With the development of nanotechnology, microchips with sensors for specific molecules could be attached to teeth, dentures or braces as an aid to diagnosis and to monitor the progress of treatment regimes.

The following "roadmap" illustrates the likely progression of some of the fields of research listed above (see Fig. 5.3.9). Synchrotron and neutron aided research are expected to play an increasingly important role.

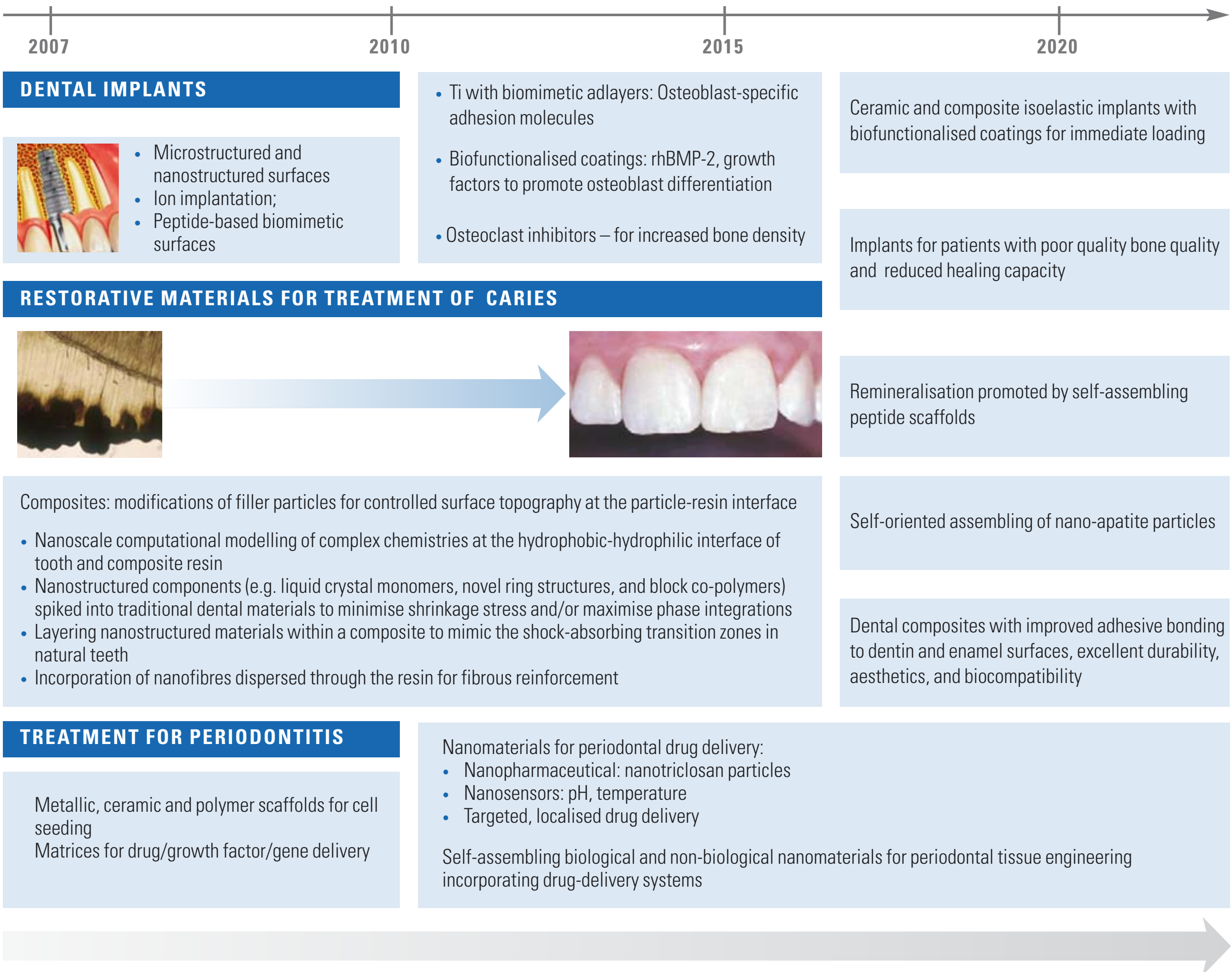


Fig. 5.3.9: Roadmap illustrating the likely progression of relevant research in dentistry.

Research topics in which synchrotron radiation and neutrons will play an important role in the future research

1. Biomineralisation – understanding enamel formation

Biomineralisation is the process by which living organisms produce inorganic crystalline or amorphous mineral-like materials from supersaturated ionic solutions through controlled deposition and regulated growth. The desire for technological advances to allow control of features in hierarchical systems from the nanometre scale to the macroscopic scale drives the need to understand such processes. In terms of regenerative medicine this will aid the development of innovative therapies to repair, replace, or restore function in organs and tissues impaired by disease or injury.

During biomineralisation proteins act as nucleators or inhibitors in cells or extracellular matrices and the precise role of these proteins determine the formation of the mineral phase. Dental enamel is recognised as being an excellent model for the molecular dissection of matrix-mediated biomineralisation events. It therefore provides an excellent model for biomineralisation in a hierarchical biological apatite structure. Certain proteins are known to be associated with enamel formation; in particular amelogenin is known to play a major role.

Neutron aided research

1. In-situ neutron reflectometry (NR) to study the protein/mineralisation front interface with sub-nanometre resolution;
2. NR to study the protein/implant interface in implant materials e.g., fibronectin adsorption onto biological apatite.

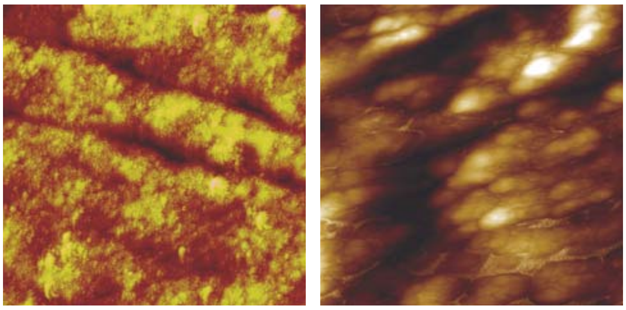


Fig. 5.3.10: The image on the left shows an AFM image of polished ivory, while the image on the right shows an AFM image of ivory fibronectin adsorbed for 24 h at 4°C, then air dried.

2. Amelogenesis Imperfecta

Amelogenesis imperfecta (AI) describes a common group of inherited genetic defects of dental enamel that affect the amount, composition, density and structure of the enamel formed. There are at least 14 different sub-types of AI. Of these subtypes, hypomaturation AI presents enamel which appears to be the most compositionally different to healthy enamel. It is characterised clinically by enamel of normal thickness that is hypomineralised, mottled, and detaches easily from the underlying dentin. We can inform diagnosis and design potential treatment regimes for patients by understanding the basic crystallography of dental enamel affected by AI and relate this to the structural phenotyping of the enamel.

Synchrotron aided research

- Nanoscale probing of texture and composition in intact sections of teeth affected by AI;
- 2-D texture and composition distribution maps of AI teeth.

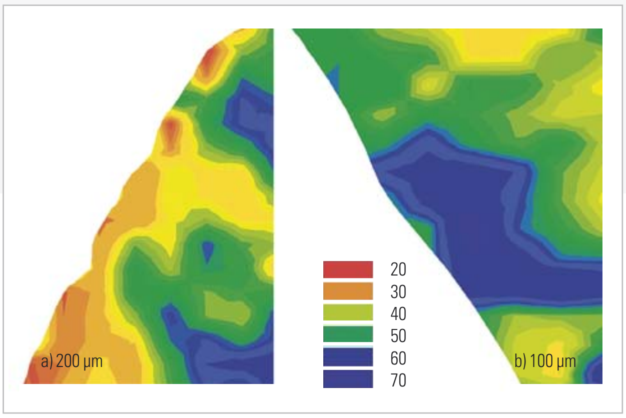


Fig. 5.3.11: Texture distribution as a function of position in a) healthy deciduous enamel (left), and b) deciduous enamel affected by hypomaturation amelogenesis imperfecta (right). The colour scale corresponds to the texture coefficients (arbitrary units) generated from Rietveld refinement of synchrotron x-ray diffraction patterns – the higher the coefficient the more ordered the enamel crystallites.

3. Repairing bone and soft tissue

3.1. Biodegradable nanofibrous membranes that mimic the natural extracellular matrices of the oral mucosa can be used to segregate different cell populations in healing tissues, for example to prevent epithelial cell overgrowth and promote bone-forming osteoblast differentiation in a periodontal defect. In advanced periodontal disease both the periodontal ligament and the bone may be destroyed and the regeneration of these tissues presents a difficult challenge, but one that may be overcome by the use of tissue engineering, using three-dimensional nano-fibrous scaffolds to promote independent development of the adjacent hard and soft tissue cell populations.

3.2. Bone graft substitute materials

Synthetic bone graft substitute materials can be used to replace bone that has been damaged by trauma or disease, for example in a periodontal pocket formed as the result of periodontitis or following tooth extraction. They may also be used to augment the alveolar bone in order to place a dental implant when the patient's own bone is insufficient. Synthetic bone should mimic the architecture of natural bone to allow vascularisation as well as osteoblast differentiation within the artificial matrix. Ideally, the material should be osteoinductive (inducing bone formation) as well as conductive (permitting bone to grow up to the surface) and have similar mechanical properties to the adjacent bone to avoid stress-shielding. Nanoscale biomaterials, with pores or crystals of less than 100 nm can promote osteoblast differentiation whilst materials which consist of nanoscale grains should have superior mechanical properties in comparison with materials with larger grain sizes. Currently bone-substitute materials can only be used to repair small defects in non-load-bearing applications.

Composite nanomaterials which, like bone, consist of an elastic matrix and an inelastic mineral (carbonate-substituted hydroxyapatite) component may overcome the mechanical problems and enable artificial bone to replace larger defects anywhere in the body.

Synchrotron aided research

Bone and soft tissue scaffolds and tissue-engineered bones can be analysed by x-ray microtomography and x-ray microdiffraction to show:

- The arrangement of trabecular and cortical bone;
- Integration/resorption of bone-graft substitute materials;
- The interface between a dental implant and bone.

Direct dental restorations

Dental caries begins in early life and affects more than 80% of the adult population by the age of 18 in the UK and USA. Currently the only treatment is to remove the decayed tissue and to fill the cavity with an inert material that blocks further decay. Mercury-containing amalgam used to be the material of choice for molar teeth but in many countries this is being phased out in favour of white composite materials which are aesthetically superior and have no toxic components.

The desire to replace amalgam fillings has meant that the use of adhesive techniques in dentistry is rising and has resulted in the increasing clinical use of a glass-filled polymeric material, known as dental composite. These white composite materials are cured in-situ typically upon application of light of a suitable wavelength that causes an addition polymerisation reaction via free radicals to bring about setting. The polymerisation process causes a reduction of the free volume of the composite. This shrinkage can result in stresses being set up in the adjacent tooth structure. We can improve the placement of restorations and the composite materials used by understanding the interplay between the basic crystallography and the mechanical properties of enamel in healthy teeth as compared to restored teeth.

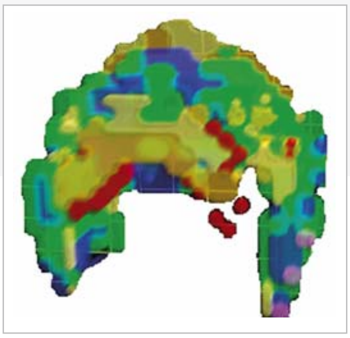


Fig. 5.3.12: 3-D reconstruction of texture distribution in human lower premolar dental enamel created by Rietveld refinement of synchrotron x-ray diffraction patterns.

Synchrotron aided research

1. Combined synchrotron XRD/XRF to study strain, texture, lattice parameters, composition in healthy and restored teeth to create 3-D maps of texture, strain and composition;
2. In-situ filling/loading synchrotron XRD studies to measure the change in strain in enamel during and following restoration placement;
3. 3-D imaging of dye leakage test substances to test for micro-leakage around restorations;
4. In phase composites x-ray tomography to study interpenetration of phases.

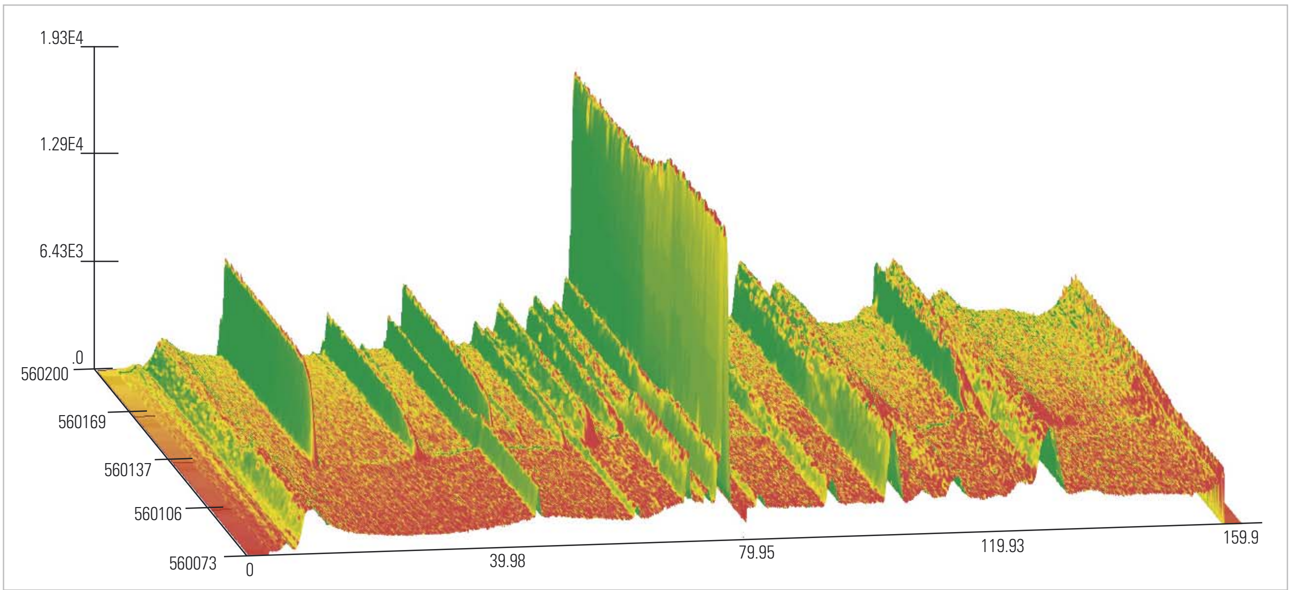


Fig. 5.3.13: Crystallisation of a fluormica glass-ceramic observed by kinetic neutron diffraction.

Indirect dental restorations

The production of crowns and inlays through Chairside CAD-CAM technologies represents a potential paradigm shift in dental treatment. Materials suitable for such restorations must be strong, tough yet machinable. At the University of Leeds a series of mica based glass-ceramics has been developed and kinetic neutron diffraction has been used to uniquely follow the crystallisation of these materials. It has been observed that the materials crystallise to the expected mica phase via an unstable intermediate phase and been shown that the crystallisation of such materials is robust in terms of changing temperatures and times of crystallisation.

Neutron aided research

1. The high penetration of neutrons, coupled with a high flux allows the bulk crystallisation of mica glass-ceramics for dental restoration to be uniquely followed in real time in beam using a combination of SANS and kinetic neutron diffraction.

2. This technique has also been used to look at crystallisation of apatite containing glass-ceramics with potential applications as bone substitutes. These materials can be cast (apatite-mullite) or machined (apatite-mica) and have applications in maxillofacial surgery and beyond.

Imaging of teeth

The dentine of teeth consists of fluid containing dentinal tubules radiating from the pulp. If tubules are exposed, they provide a potential pathway to the pulp for bacteria which can result in the loss of the tooth. The principal requirement for any dental restorative procedure is thus to seal these tubules, preventing bacterial ingress.

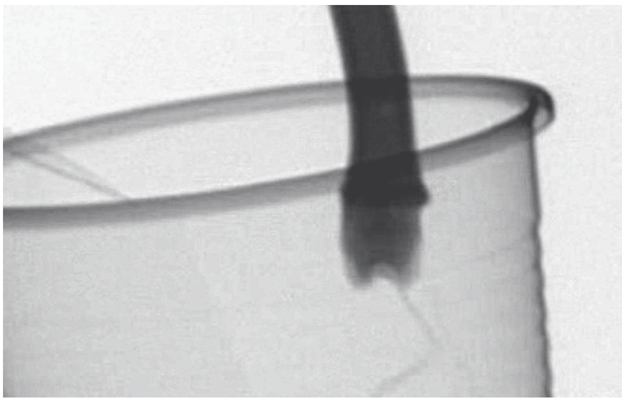


Fig. 5.3.14: Neutron tomographic image of fluid flow through a premolar tooth.

Neutron aided research

Using the contrast between H_2O and D_2O, neutron tomography will allow us to assess the permeability of dentine after various treatment modalities.

Research areas in which synchrotron radiation and neutrons will play an important role in the future

1. Regeneration of the periodontal tissues (cementum, periodontal ligament and bone) for repair of periodontal defects. In order to do this we need to understand how these tissues generate in the embryo and how they may regenerate following injury and how different tissues communicate with each other, both in terms of growth and development and in terms of mechanical stress transfer. For this we need molecular probes for growth factors and other signalling molecules. We need improved microscopical techniques which will allow us to measure molecules at interfaces and the ability to resolve microscopic environments in their natural state, using soft (destruction free) probes for organic, biological molecules.

2. Caries will (probably) always be a problem but we need to detect it at an early stage whilst remineralisation is still a possibility and before decay progresses to the dentine and beyond. For this we need better molecular probes to detect the bacteria which lead to decay and to eliminate them, and methods to promote remineralisation, involving protein-directed biomimetic self-assembly mechanisms, that can be followed in real-time experiments.

3. If, despite everything, caries occur, then we need to have filling materials with excellent aesthetics so that they are indistinguishable from the natural tooth, last the lifetime of the patient and have similar mechanical properties to those of the original tooth, so that they can be used for front teeth as well as in less visible areas of the mouth. Interpenetrating nanophase composites show great promise in this area. To develop these we need to understand the chemistry at the interface between the different component phases and between the material and the tooth. This requires better spacial resolution and the ability to do real-time experiments, for example to follow setting reactions and to show that microleakage around a filling does not occur.

4. Developing biomimetic dental implants that promote osseointegration even in patients with poor bone quality & reduced healing capacity. Rapid advances are being made in dental implant surface technology in order to provide surfaces that the cell "sees" as a natural extracellular matrix and which provide signals for cell differentiation and thus actively promote osseointegration. But what actually happens at the interface between the implant surface and bone is currently very difficult to study. What is required is probes that "see through" bone to the buried interface and detect specific molecules there, that can only be achieved with synchrotron and neutron scattering. Such bone-graft interface research is relevant, not only to dentistry and the repair of periodontal bone, but to all situations in the body where damaged bone needs to be replaced and where we want to use an artificial material rather than using the patients own bone and thereby causing further pain and putting another part of the body at risk of infection.

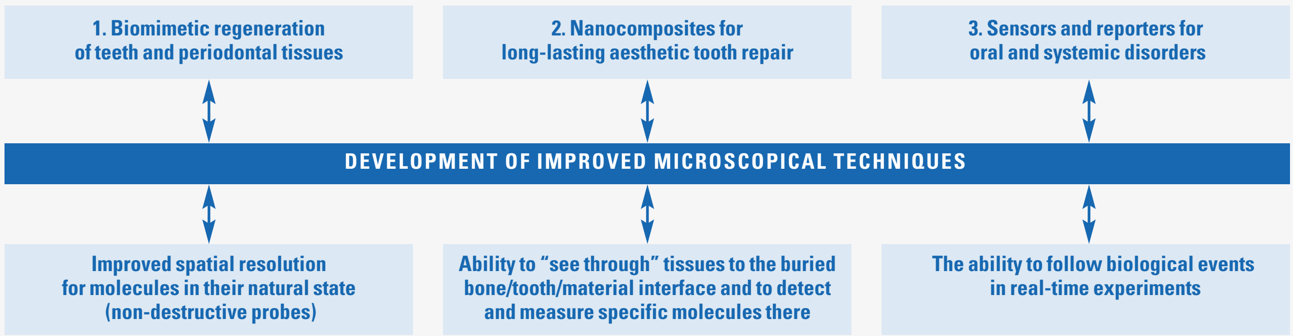


Fig. 5.3.15: Major research areas in which nanotechnology and synchrotron radiation and neutrons will play important role in dentistry in the future.

Summary and recommendations

To achieve the goals described above, we need:

- **Improved public awareness:** "What can the synchrotron and neutron sources do for us?"; Improved links to research councils with active promotion: roadshows, web links, away-days, etc.
- **Improved and simplified access** to all the large-scale facilities, Europe-wide. This could be facilitated by:
  - Allocation to the dental- bio-nanomaterial researchers community a guaranteed number of days access to instruments in both neutron and synchrotron facilities, managed by an internal community peer review process (as with major research council grant applications) and with suitable support staff and laboratory facilities.
  - Promotion of schemes facilitating access to cross-discipline teams to encourage collaboration between clinicians, scientists and industry.

- **Improved technical capabilities,** which should include:
  - Nanofocused diffraction instrumentation
  - Fast detectors (for either/both neutrons/synchrotron x-rays, with a variety of sample environments, including:
    - Controlled temp and humidity;
    - Hydrothermal treatment vessels;
    - Nano-manufacturing techniques in-situ, in beam;
    - Improvements in the resolution of detectors for neutron tomography.

All these technologies are currently being developed and we look forward to having the opportunity to use them.

5.3.4. PHARMACEUTICALS

The introduction of nanotechnology in pharmacology ("nanomedicine") has revolutionised the delivery of drugs, allowing the emergence of new treatments with an improved specificity. Nanotechnology is now widely implanted in the development of drug delivery methods. These new nanodevices can be tailored according to the desired functions and duties thanks to parallel progresses in the synthesis of colloidal systems with controlled characteristics. These systems are exploited for therapeutic purposes to carry the drug in the body in a controlled manner from the site of administration to the therapeutic target. This implies the passage of the drug molecules and drug delivery system across numerous physiological barriers (i.e. epithelium, endothelium, cell membrane), representing one of the most challenging goals in drug targeting.

Key research areas in nanotechnology for medicine are:

- the control of the drug release and distribution;
- the enhancement of drug absorption (by mucosa or cells);
- the protection of drugs from degradation.

Research roadmap for nanopharmaceuticals

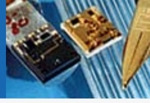
First generation of nanopharmaceuticals

An understanding of the in vivo interaction of nanotechnologies i.e. liposomes, nanospheres, nanocapsules, ultrasmall iron oxide particles etc. with biological fluids has led to the tailoring of systems which are efficient, after intravenous administration, in targeting the macrophages of the reticuloendothelial system (the Kupffer cells of the liver or the macrophages of the spleen and of the bone marrow): Fig. 5.3.16. This specific tissue and cells distribution is explained by the opsonisation processes which occur at the surface of these carriers (Fig. 5.3.16). Therapeutic applications of these systems include i.e. the treatment of cancer liver diseases.

Second generation" nanocarriers

Avoiding the recognition by the liver and the spleen is also possible by developing long circulating nanocarriers ("stealth" or able to avoid the opsonization process and the recognition by the macrophages). The design of such carriers is based on the physico-chemical concept of the "steric repulsion": by grafting polyethyleneglycol chains at the surface of the nanodevices, the adsorption of seric proteins may be dramatically reduced due to steric hindrance. Such an approach allows maintaining the drug carrier for a longer time into the circulation and the resulting extravasation towards non reticuloendothelial-located cancers may become possible.

New applications and exciting perspectives are proposed for the delivery of drugs to previously non accessible diseased sanctuaries, like the brain (treatment of glioma and autoimmune diseases of the brain)



or the ocular tissues (treatment of the autoimmune uveitis). In these specific diseases, the production of cytokines makes the vascular endothelium dramatically permeable to certain types of nanoparticles, which open options for new medicines. It is not questionable if new research programs are needed to better understand the role of cytokines on the endothelium permeability as well as the influence of the molecular coverage of the nanoparticles on their extravasation ability. From those researches, more rationale strategies for the targeting of inflamed tissues should emerge.

Third generation nanotechnologies

These allow the efficient targeting of cells reacting to certain receptors, markers and/or antigenic determinants. As an illustration of this approach, folate decorated liposomes or nanoparticles were found to recognise in a highly specific manner cancer cells with hyper expression of the folic acid binding protein. Thus, nanomedicines offer so many advantages to improve the precision of the treatment that some were marketed during the last decade.

Barriers in nanopharmaceuticals

So far, there is still no universal platform suitable for the delivery of all kinds ofdrugs. Moreover, current nanotechnologies have important limitations due to:

- A poor drug loading which is usually less than 5% (weight % of the transported drug versus the carrier material). Thus, nanotechnologies apply only for compounds active at very low dose;
- The rapid release (so called "burst release") of the encapsulated drug after administration, generally corresponding to the release of the drug fraction which is simply adsorbed (or anchored) at the surface of the nanocarrier;
- The difficulty to design synthetic materials with low toxicity, sufficient biodegradability, absence of cell/tissue accumulation and lack of immunogenicity.

There is, therefore, an urgent need for new ideas and concepts able to impact drug delivery processes and allowing the discovery of breakthroughs.

Research to be encouraged

- To develop nanomedicines with high drug loading;
- To introduce new, more efficient and safer (bio)materials for drug targeting purposes;
- To use natural or biomimetic compounds;
- To develop nanomedicines with controlled release at the site of the disease; to improve drug's therapeutic index, to fight resistances to drug treatment, since resistance is a major concern that maybe overcome using "intelligent" nanodevices;
- To combine multifunction nanoparticle capabilities with drugs, enabling in vivo monitoring and directed transport of drug agents;
- To engineer tailored release dynamics for drugs by manipulating surface and bulk properties of drug nanoconstructs;
- To evaluate and optimise drug transfer through cell compartments effective therapeutics with reduced adverse effects;
- To contribute in the rejuvenation of the pharmaceutical industry by providing new and high-quality technology and valuable IP;
- To bridge the gap between traditional pharmaceutical technology (e.g. tableting, injectibles of small molecules) and biotechnology (e.g. monoclonal antibody and peptide therapeutics);
- To develop nanotechnology techniques and tools (AFM, SPM, X-ray fluorescence) which will need be used in the characterisation of nanopharmaceuticals, providing regulatory authorities (EMEA, FDA) with new information regarding their properties and stability;
- To determine body deposition through the use of dynamic, real-time imaging of nanopharmaceuticals;
- To combine advanced nanopharmaceuticals with electrical and electronic engineering components in order to allow information transmission and reception capabilities;
- To combine nanopharmaceutical materials with traditional pharmaceuticals with devices such as catheters, endoscopes and needles which have the capacity to release specific dosage forms of pharmaceuticals;
- To have a clear toxicity profile (see also Section 5.10. Toxicology) so that the risk-benefit analysis will favour the benefits.

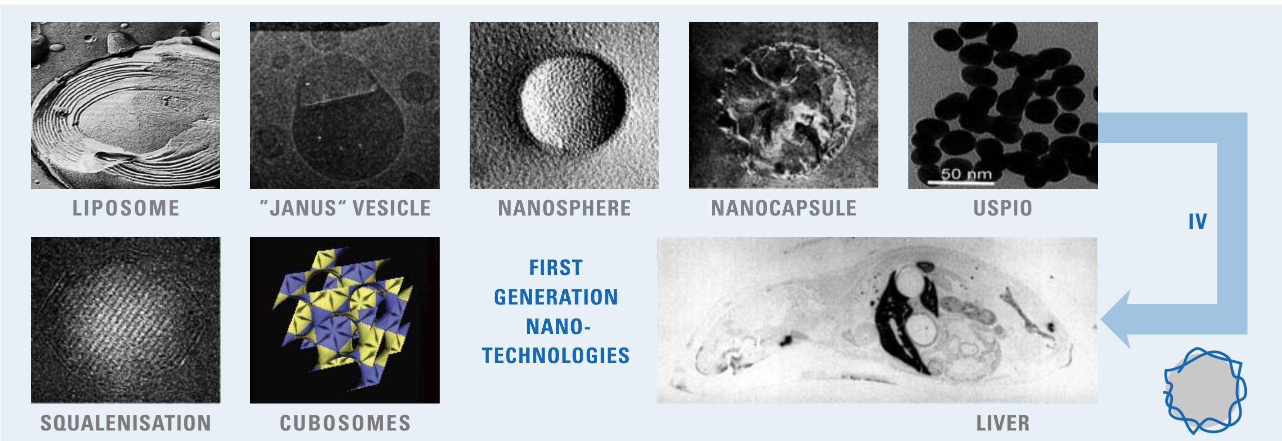


Fig. 5.3.16: First generation nanotechnologies (ie. liposomes, polymer nanospheres and nanocapsules, iron oxide nanoparticles etc.) concentrate in the liver due to the adsorptionof blood proteins (blue) at their surface.

5.3.5. HEALTHCARE, COSMETICS, OINTMENTS

Nanomaterials for the cosmetics industry

The sources of nanomaterials are multiple: i) biological (milk: casein micelles, viruses), ii) natural (volcanic ash, erosion), and iii) man-made (diesel exhausts, manufactured nanoparticles). Typical formulations of nanosized cosmetics are: liposomes 120 to 250 nm), nanocapsules (120 to 500 nm), nanoemulsions (up to 50 nm), and oleosomes (120 to 400 nm). The principle features affecting physical and biological properties of nano- or microparticles are: i) quantum effects: especially important at the low end of the nanoscale and may produce changes in optical, magnetic, thermal properties; ii) increased surface area per unit mass which may affect dissolution kinetics, bioavailability or increased surface activity.

From the Egyptian era onwards, nanotechnology has been used to prepare make-up or skincare products. Today's cosmetic industry has long been a user of nanotechnology to improve its products with enhanced properties. Many scientific fields are involved:

- Physics and materials science for optical properties, e.g. UV-absorption, interferential effects;
- Organic and physical chemistry for controlled release of molecules, and self-assembly of soft matter;
- Biology for bio-inspired (biomimetic) materials.

When considering a given mineral for cosmetic use, a wide variety of product properties are attainable by altering its different parameters:

- Particle size and morphology;
- Crystallinity: amorphous state or allotropes, crystalline domain size;
- Surface state: controlled from the synthesis protocol and further functionalisation;
- Mixed phases and doping;
- Core-shell structures.

As far as soft matter is concerned, self-assembly properties and interactions between functional groups and inorganic surfaces may display significantly different physical behaviour (optics, rheology) with only small variations in their composition, which allows the tuning of some target properties through appropriate formulation.

State of the art of nanosized cosmetic materials/substances

Mineral materials

Minerals can have both protective and decorative functions within products:

1. Today, the most well-known products are sunscreens that contain nanoscale titanium dioxide or zinc oxide particles. These compounds:

- Provide UVA- and UVB-protection;
- Are transparent because of their nanosize and do not cause visible whitening on application of the lotion;
- Are used extensively in foundations which need UV-protection for people with sensitive skin profiles.

Titanium dioxide is a mineral UV-filter composed of microsized aggregates. The aggregates themselves are composed of grains which are nanosized. These aggregates are coated with a layer of silica.

2. A recent development is the use of a dopant in a common inorganic compound. A typical case: the insertion and/or substitution of iron atoms in the crystallographic structure of titanium dioxide microsized particles, induces an interesting effect called "photochromism". This kind of product is able to change its colour according to changes in lightning.

3. Additionally, interferential effects have great use in make-up products. These effects are based on the difference of optical index between material layers. Therefore, control of layer thickness and optical index results in materials changing their colours according to the observation angle.

Organic materials

In 1985, the cosmetics industry introduced nanotechnology-based products that used the self-assembling properties of phospholipids to adjust the biodisponibility of active ingredients. This was the birth of liposomes in the cosmetic industry, which have now become common ingredients in topical lotions.

Thus, various self-assembling systems have been developed using amphiphilic block copolymers, supramolecular systems, surfactants, etc. and have provided more and more complex structures and improved rheological properties.

Hybrid materials

The cosmetic market is proposing products from hybrid nanotechnology i.e. organic/inorganic UV-filter, the basis for innovation now includes:

- The use of organic compounds to modify the inorganic surfaces of pigments;
- Active ingredient encapsulation in an inorganic shell to transport it.

One of the most interesting applications of hybrid materials is to obtain surfactant-free emulsions, so-called Pickering emulsions. Around 1910, Pickering prepared paraffin/water emulsions which were stabilised merely by the addition of various solids, such as basic copper sulphate, basic iron sulphate or other metal sulphates. For this type of emulsion, Pickering postulated the following conditions:

- The solid particles are only suitable for stabilisation if they are significantly smaller than the droplets of the inner phase and do not have a tendency to form agglomerates.
- An important property of an emulsion-stabilising solid is its wettability. In order to stabilise an emulsion, the solid has to be more readily wettable by water than by oil.

Today, development of hybrid materials and of surface functionalisations allows us to bring amphiphilic properties to particles, which is one of the key factors to obtain Pickering emulsions. This is because, without particle surface functionalisations, the affinity for both phases would be too different to allow for stabilisation by absorption in the interfaces of closely packed solid particles.

A large variety of emulsions can be prepared: direct emulsion, inverse emulsion, double emulsion, ..., and also a large variety of modified surface particles can be used such as: talc, silica, titanium oxide, fat crystals, and of course a large variety of functionalisations with: dimethylpolysiloxane, octylsilanol for hydrophilic particles and polymethylmethacrylate, polysaccharides, metallic oxide for hydrophobic particles.

The potential of nanocosmetics

Design of new nanomaterials

Nanomaterials can be the basis for new multifunctional materials and for active or smart products:

- Improvement of psycho-sensitive properties, such as soft touch and controlled release of active ingredients;
- Easier application and removal;
- New materials with unexplored optical properties offer significant potential:
  - Solid solutions,
  - Amorphous state,
  - Multiscale materials;
  - New organic/inorganic hybrid materials.

Nanotechnology-based innovations

The directions for improvements are focused on:
i) Nanoemulsion technology: unique textures, transparency i.e. hair conditioner;
ii) Nanocapsule technology: protects active ingredients in i.e. skin care;
iii) Nanopigment applications: UV-filters, consumer compliance i.e. sunscreen.

Target: "Design of cosmetic nanomaterials"

Realistic aims for the development and introduction of cosmetic products featuring nanotechnology-derived properties include:

- Improved UV-filters:
  - Thanks to morphology tuning, integrating surface state considerations to increase the state of dispersion and coverage when applied.
- New inorganic photochromic materials:
  - Better knowledge of mechanisms and reversibility kinetics, controlled defect creation on the surface or in the core of particles, distribution of the dopant and multiple doping.
- New thermochromic materials:
  - Intense colour change around human body temperature with a delta near one degree Celsius.
- Materials responding appropriately to a stimulus from the surroundings:
  - Release of protective molecules from capsules under light, heat or other excitation.
- Materials obeying user specific actions:
  - Colour change or molecules released by light, magnetic field or ultrasound; this implies co-development of materials and specific "pencils".
- New formulations to take advantage of self-organisation during application or drying:
  - Coverage for solar filters, lotus effects, colloidal crystals...

Role of synchrotron radiation and neutron

Synchrotron radiation and neutron facilities will play an integral role in the development and design of new nanomaterials and technology for cosmetics and the understanding of the mechanisms during exposures. Research ideally suited to synchrotron radiation and neutrons include:

- Characterisation of doping at the atomic level (crystal sites) or nanometric level (clusters formed by dopants) and of solid solutions;
- Characterisation of interactions between inorganic surfaces and organic matter;
- Description of local self-assembly in complex formulations;
- Kinetics of controlled release by capsules;
- Observation of formulation constituents by IR-microscopy thanks to synchrotron sources.

STATE-OF-THE-ART

Passive materials
- Pigments, dyes
- UV-filters
- Capsules with kinetically controlled release

Smart materials
- Photochromic particles

FUTURE PROSPECTS

Passive materials
- UV-filters: simultaneous optimisation of particle size and morphology, surface treatment and self-assembly for better coverage.
- New interferential effects based on colloidal crystals.

Smart materials
- New thermochromic materials applicable to cosmetics.
- Appropriate change in response to stimuli: fast and reversible darkening under illumination, release of protective molecules from capsules under temperature increase...
- Materials obeying to user's wishes: colour change by light or magnetic pencils, easy application and removal.

FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRONS SOURCES

- Characterisation of doping, solid solutions and amorphous state.
- Description of organic/inorganic interaction and hybrid materials.
- Characterisation of phenomena occurring during application, drying or under light, magnetic or ultrasonic stimulation.
- Characterisation of self-assembly and self-organisation phenomena.

Fig. 5.3.17: Roadmap for nanomaterials in the cosmetic industry.

Nanotechnology in skin delivery: pharmaceutics and cosmetics application

The skin covers a total surface area of approximately 1.8 m^2 and provides the contact between the human body and its external environment. This outermost layer of the human body, see Fig. 5.3.18, is easily accessible and hence attractive as a delivery route. Dermal drug delivery is the topical application of drugs to the skin in the treatment of skin diseases, and has the advantage of high concentrations of drugs at the site of action, reducing side effects related to systemic drug concentrations. Transdermal drug delivery uses the skin as an alternative route for the delivery of systematically acting drugs.

The advantages of transdermal delivery are that it:

- Circumvents the variables that could influence the gastro-intestinal absorption such as pH, food intake and gastro-intestinal motility.
- Circumvents the first-pass hepatic metabolism and is therefore suitable for drugs with a low bioavailability.
- Results in a constant, controlled drug input, thereby reducing modulations in drug plasma levels. For drugs with a narrow therapeutic level this will result in a reduction of side-effects.

There is one major challenge in skin delivery, namely the low permeability of human skin for most drugs. Compounds are delivered via the appendages (such as hair follicles) or via the transepidermal route.

State-of-the-art: nanomaterials

The physicochemical characteristics of nanomaterials have a large effect on the efficiency of:

- Follicular delivery showing that smaller particles less than 1–2 µm are more efficiently transported along the hair follicles than larger particles, typically larger than 2 µm, see Fig. 5.3.18 – 5.3.20.
- Interfollicular delivery. The main barrier of the skin resides in the outermost layer of the skin, the stratum corneum, see Fig. 5.3.18. The highly organised crystalline lipid lamellae play an essential role in the barrier properties of the stratum corneum. Nanoparticles as skin delivery systems are attractive, especially when the vesicles are highly elastic (low interfacial tension).

A wide variation of lipids, surfactants and polymeric entities can be used to prepare nanoparticles, very similar to those used in the food industry. The composition of the nanoparticles influences their physi-

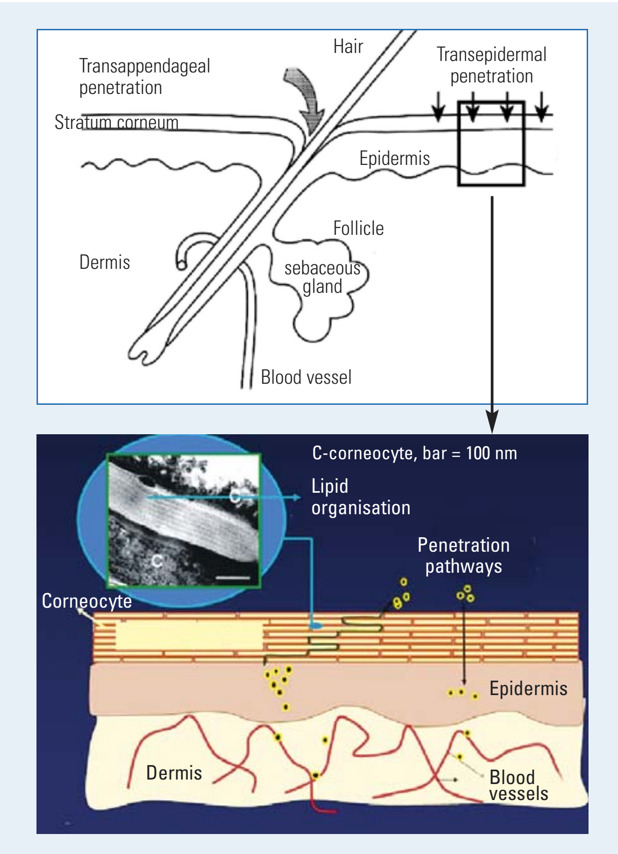


Fig. 5.3.18: The penetration routes across the skin are either via the hair follicles (appendages) or via the transepidermal route. The latter plays a major role as the total skin surface comprising of hair follicles is only approximately 0.1%.

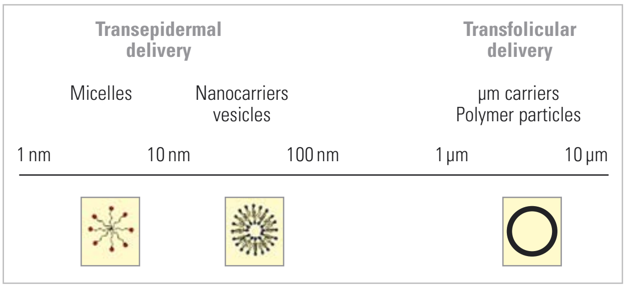


Fig. 5.3.19: Nanoparticles act as either as carrier systems, suppliers of penetration enhancers or as depot systems for drugs.

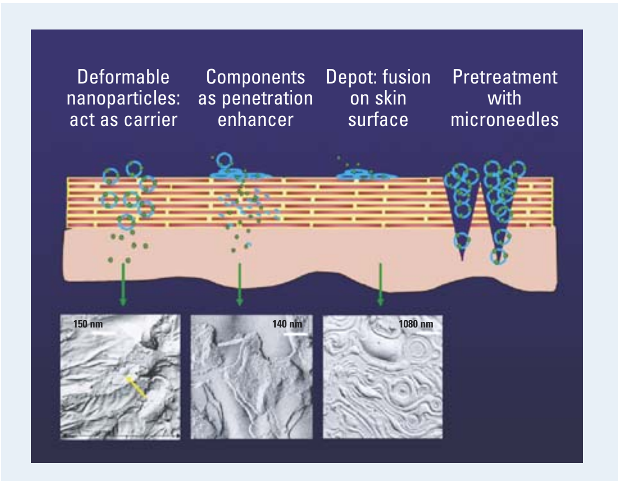


Fig. 5.3.20: Mode of action of nanoparticles in the stratum corneum.

co-chemical characteristics such as size, charge, thermodynamic phase, lamellarity and bilayer elasticity.

These physico-chemical characteristics will have an effect on:

- Drug release;
- Interaction with the skin;
- Stability issues.

Nanoparticles having a low interfacial tension have been shown to act as a carrier system (Fig. 5.3.20) and deliver drugs including biologics across the stratum corneum. Rigid vesicles (high interfacial tension) fuse on the skin surface.

Future trends of nanoscience in skin delivery

Despite extensive research and a high level of interest from the pharmaceutical and cosmetic industry, the use of nanoparticles has not yet been fully explored. For the next 12 years, at least four major breakthroughs in the skin delivery field are expected, especially taking into account the important role of biotechnology in future drug development. A road-map is provided in Fig. 5.3.21.

• Delivery of vaccines across the skin using nanomaterials

Nowadays, most vaccines are delivered by injection. However, there is an urgent need for non-invasive delivery routes, as the number of vaccines are increasing, and in paediatric vaccination programmes only a limited amount of injections are permitted per year. Vaccination via the skin is of interest as the skin is populated with a high number of dendritic cells, which makes this delivery route a very efficient one. Nanoparticles will play an important role to i) formulate antigens (active component of a vaccine) as these particles can protect the antigen from enzymatic degradation and ii) to increase the uptake in dendritic cells to initiate an immune response. Elastic vesicles have already shown their potential in this field of research (low interfacial tension).

• Targeted delivery of nanoparticulate carriers to potentiate immune response

Furthermore, nanoparticles can be tailored by adjuvants to potentiate the immune response. In order to selectively enhance the uptake in dendritic cells (cells required to initiate the immune response), nanomaterials can be modified by transporter peptides and mannose groups. Delivery of proteins (a more general term is biologics) across the skin can be done by using nanocarriers. This will be a very important field for future research, as the role of biotechnology in the development of drugs is growing rapidly. In general, due to their limited physico-chemical stability and rapid enzymatic degradation, biologics cannot be administered by the oral route due to degradation of the protein. Therefore, they will be administered either by injection or by alternative delivery routes, such as via the skin. When administered via the skin, nanoparticles will play an important role in protecting these drugs.

• Gene delivery via the skin

The accessibility of the skin makes it a very attractive route not only for DNA vaccine delivery, but also to repair skin diseases. With the increasing knowledge on the role of gene mutations in various skin diseases, this will be an important challenge for the future. A well-known example is atopic dermatitis. Currently 20% of the children in the western world suffer from atopic dermatitis. For many years it was thought that this disease was of immunological origin. Very recently, it has been established that the disease is caused by a gene mutation in filaggrin, a protein playing an important role in the skin barrier. Gene repair will be an important issue in future treatment of atopic dermatitis. One of the most important delivery systems for DNA and RiRNA are nanomaterials. Although some research has already been carried out to characterise the delivery systems, the role of synchrotron radiation and neutron scattering has hardly been explored.

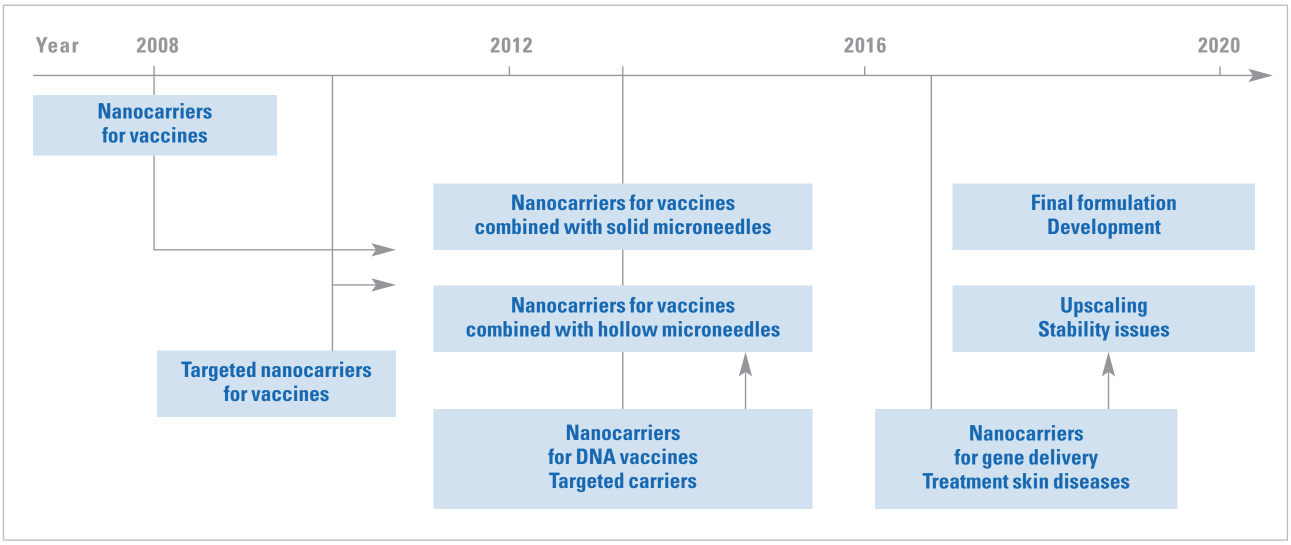


Fig. 5.3.21: Roadmap for nanoscience in skin delivery.

• Combined approach nanoparticles and microneedle arrays

Microneedle arrays pierce very small conduits in the skin, thereby facilitating the transport of especially high molecular weight drugs, such as DNA, antigens and proteins across the skin, see Fig. 5.3.20. Microneedles are very short and therefore pierce the stratum corneum, but do not reach the nerves located in the dermis, therefore no pain sensation is experienced. Solid microneedles are used to pretreat the skin, see Fig. 5.3.19. When using hollow microneedles, the formulation is injected via the needle. One of the most elegant delivery systems will be a combined approach of microneedles and nanoparticles. Microneedles are used to facilitate the transport across the stratum corneum, while nanoparticles protect the drug against degradation. Surface modified nanoparticles facilitate the uptake in or targeting to cells.

Role of synchrotron radiation and neutron mediated research in nanoparticles for skin delivery systems

The role of synchrotron radiation in the development of all these new challenges in the skin delivery field can only be met when the delivery systems are fully characterised, and their mode of action in the stratum corneum and deeper viable layers is fully understood. In this process, characterisation by synchrotron radiation and neutron scattering will play a major role. In general, it should be said that most systems used until now are only poorly characterised by physicochemical methods. One of the reasons is the metastable nature of many nanoparticles used in drug delivery.

Nanoparticles

Several methods are currently used to characterise the nanoparticulate systems used in drug delivery. Among them are light scattering, electron microscopy, and several spectroscopic methods. However, x-ray diffraction and neutron diffraction are very important tools to characterise nanoparticles. Although electron microscopy has the advantage of very detailed structure information, it has the important disadvantage of specimen treatment. Furthermore, electron microscopy is very time-consuming in obtaining statistically relevant information. As the nanoparticles in drug delivery are often very weak scatterers, synchrotron and neutron facilities are crucial to determine information on the structures itself. In case of neutrons, contrast variation is an elegant tool to provide details on the bilayer structure of vesicles, but also to determine detailed information on those particles in the range of 1–10 nm.

Loaded nanoparticles

As soon as the nanoparticles are loaded with antigens or proteins, the systems become more complicated. In this case x-ray and neutron facilities play a very important role in unravelling the nature of the association between the protein or antigen and the nanoparticle. Furthermore, detailed information can be obtained on the aggregation of proteins. In formulating proteins, aggregation is a key problem which is difficult to detect. A combined approach of x-ray and neutron scattering is one of the few methods to obtain information on the domain sizes of these aggregates. This information can also be obtained from electron microscopy and atomic force microscopy; however, the visualisation methods have the disadvantage of small sample sizes. Therefore these methods are often used to illustrate the structure, not just to obtain statistical information.

Interaction nanoparticles with skin

As the stratum corneum, the upper layer of the skin, has a very characteristic lamellar organisation, x-ray diffraction is an excellent tool to study the changes in the lipid organisation as a consequence of the interactions between the nanoparticles and the skin. The change in lipid organisation can be correlated to a change in the skin barrier function and its transport rate. In addition, nowadays, various model membrane systems are available which mimic the skin lipid organisation. Using scattering methods these model membranes can be used to study in detail the interactions between nanoparticles skin lipids.

Final formulations

When designing the final formulations, additives are added. This always requires a detailed study on the interactions of additives with the nanoparticles – especially formulations prepared from vesicles require a throughout characterisation due to their metastable nature. X-ray and neutron scattering play an important role in this.

Necessary development and recommendations

- Time-resolved and temperature-resolved measurements are of great importance in unravelling the nanostructures that are used in drug delivery. Although this chapter only focuses on the skin area, this is certainly also the case for other delivery routes, in particular the oral, but also the intravenous route. Time-resolved measurements are required in order to study the interactions of the delivery system with its absorbing membranes. This might involve pH changes, ionic strength changes and temperature changes.
- Software to analyse the data need to be up to date and easy accessible. This is especially important when working in a multi-disciplinary field as not just specialists will enter the neutron and synchrotron facilities.

As we are working in a very multi-disciplinary field, staff at the facilities need to train new persons entering the field of synchrotron radiation and neutrons. These scientists often have another background. In this respect, not only at the synchrotron sites, but also after the measurements, it is indispensable to have access to specialists who support the analysis of the obtained data, using highly specialist methods. In our experience, currently, data analysis is not supported by persons working at the facilities.

5.3.6. AGRICULTURE

Future development in agriculture will strongly benefit from advances in nanoscience and nanotechnology which will:

- Increase soil fertility and improve crop quality and production by optimising and minimising the intrants;
- Provide a better knowledge of raw materials associated with agriculture;
- Optimise new processes for their transformation within the framework of the sustainable development;
- Develop slow release and efficient dosage of fertilisers for plants and nutrients and medicines for livestock;
- Provide dedicated nanosensors to monitor the health of crops and farm animals;
- Study novel magnetic nanoparticles to remove soil contaminants.

The most important nanoagricultural developments will be in nanoseeds, nanoparticle pesticides, nanofeed for animals and agrosensors.

Research needs

- Acquire knowledge of hierarchical structures in plants (from the nanoscale in the tissues to the global properties of the plant) and modelling in order to optimise their transformation (wood, 2nd generation bio fuels, fibres);
- Tailor syntheses of new nanostructured biocatalysts in order to modify the agroresources in the green chemistry context;
- Develop the smart delivery of nanosystems for prevention, improved diagnostics and treatment;
- Improve the compatibility between productivity and nutritional quality;
- Decrease and optimise the use of nanoparticles pesticides: pesticides can be easily taken up by plants if they are in nanoparticle form; they can also be programmed to be "time-released";
- Develop nanosystems for improving the biodisponibility of "healthy" biomolecules such as antioxidants, polyphenols, vitamins;
- Develop autonomous nanosensors for real-time monitoring;
- Increase the efficiency of nanostructured biodegradable materials;
- Mimic the nanostructured natural assemblies in order to build "stimulable" materials from agroresources;
- Decrease the inputs in agriculture and reduce the pollution especially in ground water; preparation of nanobased filters and catalysts to reduce pollution;
- Improve the agricultural techniques for the production of both healthy food and well-suited resources for non-food uses as materials or biofuels.

Research roadmap

The research needs claim for nanomaterials from agriculture and for agriculture:

2008 – 2012

- Study the basic science of plant and crop structure at the nanoscale;
- Understand the hierarchical structure from the nano to the supramolecular level;
- Evaluate the structure – properties relationship;
- Explore the technical uses.

2012 – 2016

- Optimise the bio-refinery and fractionation processes of agricultural products for both food and non-food uses;
- Optimise and minimise the intrants in relation with the quality of agroresources and sustainable development.

2016 – 2020

- Develop new improved multifunctional materials and healthy foods from agro resources;
- Study new nanosystems for sustainable productions in both food and non-food applications;
- Explore remote sensing techniques for selected fields by a combined simultaneous analysis of soil, vegetation and additives.

Future role of synchrotron radiation and neutron facilities

- X-ray, UV and IR microimaging and microanalysis need to be provided to investigate chemical and structural changes in plant tissues during the plant growth or when subject to environmental changes or industrial processes.
- Special sample environments have to be developed to mimic hydration, temperature adjustment and mechanical stress
- Functional imaging of enzymes action within the plant tissues;
- Access to SAXS-WAXS experimental stations has be to assured to monitor nano-objects formation and evolution;
- Dedicated time-resolved experimental stations to monitor protein and polysaccharide folding dynamics at nanosurfaces need to be developed
- (Deuterium labelled) neutron scattering and spectroscopy stations are necessary to unravel the structure and dynamics of water or other solutes in tissues and assemblies of biopolymers;
- X-ray fluorescence spectroscopy stations should be made available to monitor diffusion and dynamics of molecules within nanostructured natural assemblies.

Conclusions and European Research Strategy

The development of a future agriculture technology should ensure a sufficiently healthy nutrition to the European citizen. Moreover, a thoughtful use of agroresources for the manufacturing of synthetic materials and new biofuels could become an important source of fossil fuel energy.

All nanoscience and nanotechnology concepts have to explore which materials carry the potential to:

- Enhance an optimised and sustainable soil fertility;
- Assure that the harvested food contributes to the health of the European citizen.

This mission will be successful, if the processing and degradation mechanisms of agroproducts are understood and controlled over a full spectrum of lengths – from nano- to macro- timescales. The European large-scale facilities must contribute to this vital task by providing the necessary analytical potential to explore the relevant nanomaterials and nanoprocesses.

5.3.7. FOOD SCIENCES AND TECHNOLOGIES

Most raw materials of foods are of natural origin and as such have been built up from functioning nanosized elements. This chapter focuses on the implications of nanoscience and nanotechnologies on food, and how developments in this area may lead to greater choice and freedom for consumers. All aspects of human life critically depend on food availability. Therefore, global changes will affect food production and the foods locally available for consumption. Key drivers for research are the impact of global warming on crop production and shelf-life, dietary needs, mitigation of disease predisposition, food-mediated preventive health care, etc. These drivers will lead to specific demands on food functionality. Nanoscience and micro- and nanotechnologies will become important factors in facing these challenges. Ultimately, these developments will lead to specific demands on food functionality (see Fig. 5.3.22).

SOCIAL/ HEALTH ASPECT	FUTURE CHALLENGE	NEW PRODUCTS
· Obesity	· Low fat products	· Zero fat cheese
· Blood sugar	· Low sugar	· Soft drinks
· Ageing/ nutraceuticals	· Encapsulation	· Vitamins minerals pro/pre biotic
· Environment	· Pollution reduction	· Biodegradable, packaging
· Elderly/infants	· High protein food	· 40% protein drink
· Lifestyle	· Vegetarians	· Plant protein based meat
· Religion	· Food composition	· Gelatin replacement

Fig. 5.3.22: An overview of societal and environmental demands put on food industry.

Food as a nanocomposite material is often a complex mixture of proteins, (poly-)saccharides, fats, water, vitamins, anti-oxidants, microorganisms, colorants, and salt (see Fig. 5.3.23). From a structural point of view, food is built of different (co-) polymers (poly-saccharides and proteins) in which fillers (often fat) are dispersed. In addition, food has glass transition properties similar to rubbers and plastics. Because of

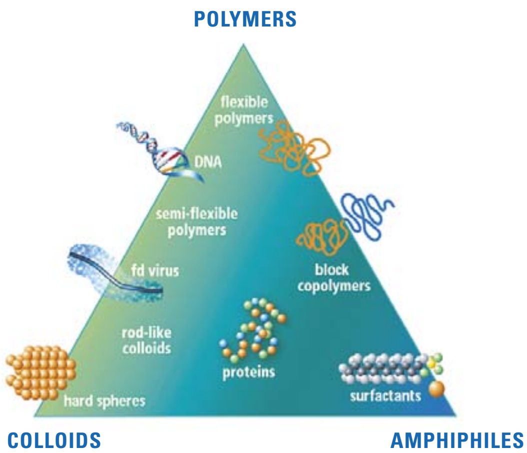


Fig. 5.3.23: Nanofood triangle.

these commonalities, it is of high relevance to study the interaction between the constituent materials, as well as the dimensional aspects, the strength, the diffusion and migration of components as done in plastic materials.

Many foods consist of structures at the nanolevel which are critical to the texture of the foods and in turn to the acceptance by the consumer. Until now, production and processing of foods has been empirical/ phenomenological and not by design. Therefore, among the future needs are systematic studies of the structure/texture of food materials including modelling/simulation, the impact of changing raw materials (due to many factors including climate change and the introduction of GM crops) and the interplay between structure and nutrition. A general scheme for food production is shown in Fig. 5.3.24.

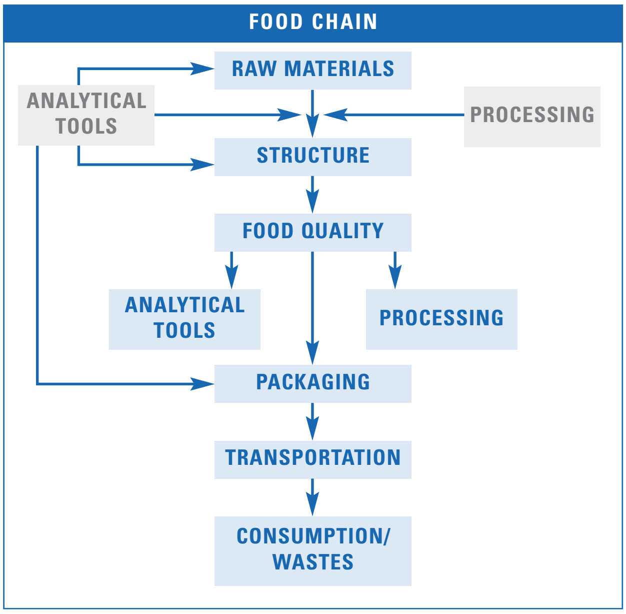


Fig. 5.3.24: Basic elements of the food chain.

The micro- and nanostructure of food which will impact nutrition include (Fig. 5.3.25):

- Nutrient release in the gastrointestinal tract (glycaemic index, satiety feeling, health benefits, e.g. protection from bowel cancer, proliferation of minerals and trace elements through gut wall);
- Nanotoxicity – it has become clear that nanoparticles can affect biological systems and the long-term effects of these particles is as yet largely unknown;
- Nutriceuticals;
- Encapsulation of flavours and vitamins;
- Food processing, packaging transportation;
- Food drying and rehydration;
- Food waste handling.

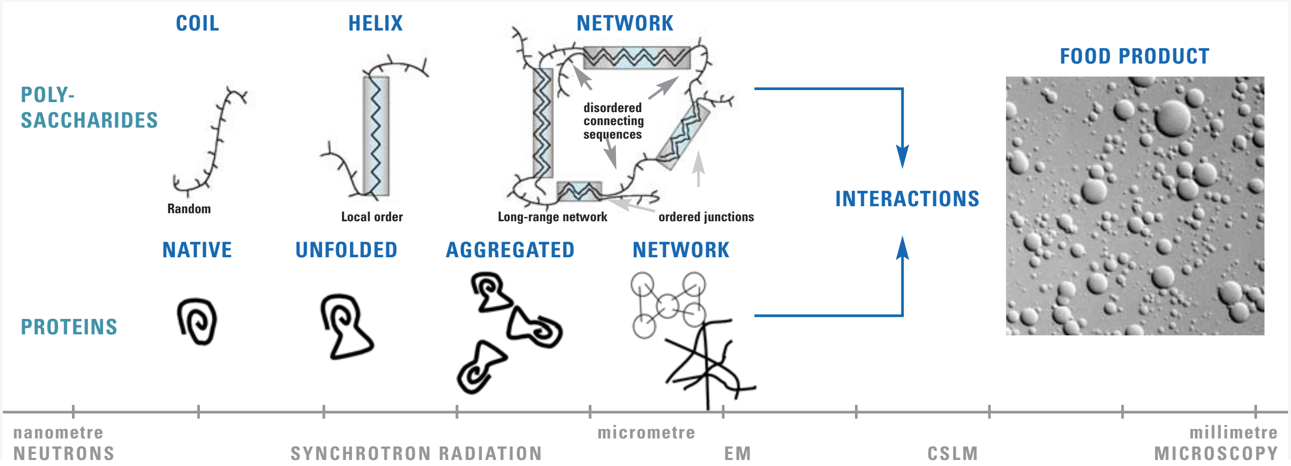


Fig. 5.3.25: The food length scale structure.

Processing must retain the safety of the food and reduce food waste and fouling by energy-efficient processes. Nanoscience can be expected to contribute to improved biosensors and rapid/online tests for food borne pathogens. Packaging is required to ensure not only protection from immediate spoilage, but also to enhance shelf-life. Nanoscience can be expected to deliver:

- Smarter packaging;
- Better biodegradability;
- New inks and barcodes for spoilage alerts;
- Enzymatic routes to the breakdown of organic material for the production of new raw materials to be used by other industries;
- Biofermentation.

Future trends in nanofood research and technology (Fig. 5.3.26)
Micro- and nanotechnology strategies are the motor for the next generation of food development. These technologies will lead to innovations in almost every field of food endeavours. The key challenges are:

- **The link between the different structures at the nano- and microlevel in food texture**
  First attempts have been made at synchrotron radiation and neutron facilities on crystallisation, phase separation, rheology and interfacial phenomena in food materials including:
  - Food additives such as thickeners;
  - Model systems such as synthetic milks, fats and gelling agents;
  - Predominantly crystalline food materials such as chocolate.

  These studies aim at correlating the micro- and nanostructure with its nutrition properties, creating a first understanding of food in terms of modern concepts of polymers and colloids, including interpretation of properties in terms of structure and interactions of polymers, of colloids and of various mixed systems.

- **Thermodynamic aspects of nanofood materials**
  Foods are usually in a metastable or unstable state. Understanding ageing, dynamic processes of physical change (such as structural

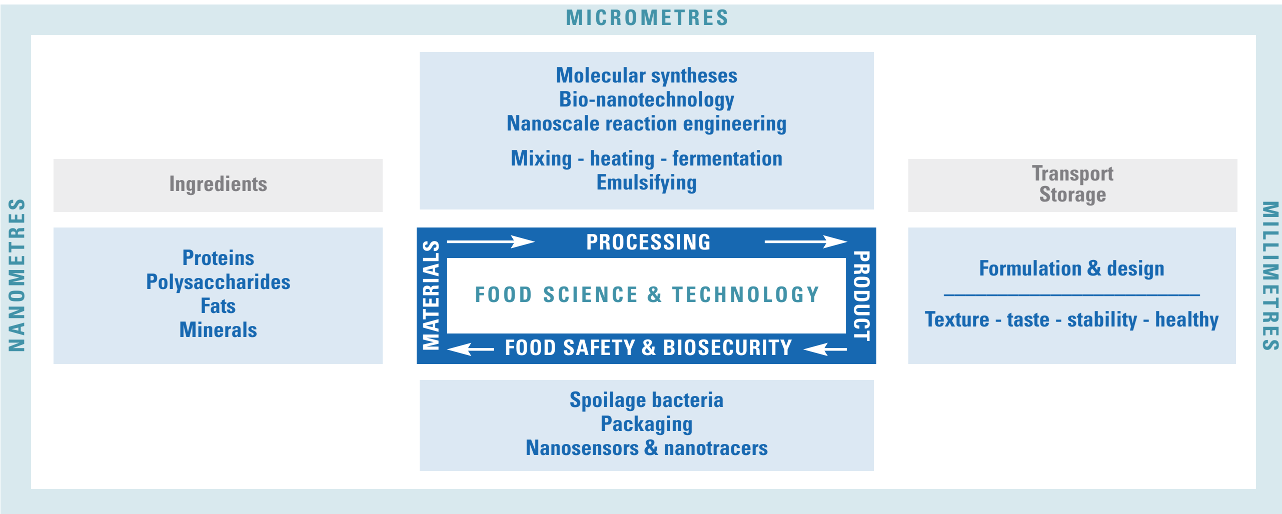


Fig. 5.3.26: Application matrix of nanotechnology in food science and technology.

transformations and crystallisation), phase separation and chemical reactions that occur on a wide range of timescales, is becoming more and more important and requires systematic and long-term studies exploiting the non-destructive in-situ capabilities of modern synchrotron radiation and neutron techniques. Understanding and control of food properties requires sophisticated measurements to identify the roles of individual components.

- **Targeted food design** (Fig. 5.3.27)
  The future challenge is to replace the empirical formulation of food by rational design for optimal functionality. Nanotechnology will allow the control of the relevant processes. To achieve these goals, basic understanding of the materials at the nanoscale is essential. New scientific impact will come from structural engineers, colloid physicists and physical chemists who understand the interaction between macromolecules, the stability of suspensions and emulsions, the structure of foams and the transport and migration of components in a complex matrix. The developments in food microbiology and nutrigenomics must now be complemented with food engineering activities.

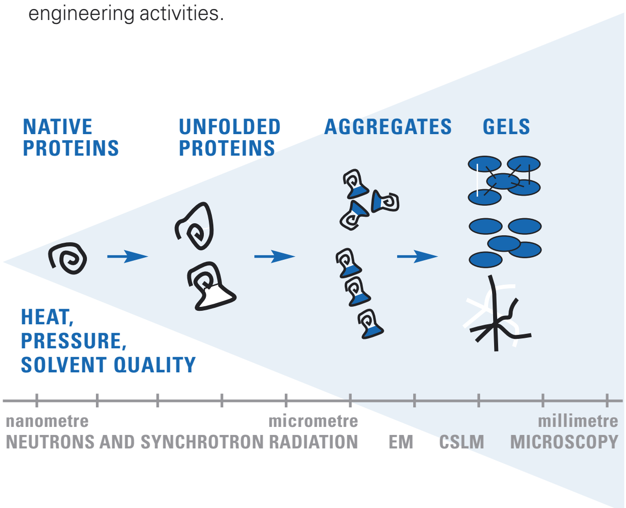


Fig. 5.3.27: Gelation of proteins in food.

- **Interaction between food and the body**
  The interaction between food and the human body is currently poorly understood. System biologists are beginning to understand better what takes place during the interaction with food using scientific concepts such as genomics, proteomics, metabolomics, nutrigenomics. The convergence of these biological sciences with nanotechnology offers opportunities to fine-tune the nutritional content of food to the actual demands of the body at any particular time, and to avoid substances that could trigger over reaction of the immune system (food allergy).

- **Nature and nanofood materials**
  Natural foods are often complex composite materials involving lipidic structures for partitioning living systems that are self-aggregating and auto-repairing, and form supramolecular assemblies. In order to exploit these bio-strategies in food nanotechnology, we need more structural information which can ideally be provided by synchrotron radiation and neutron facilities, if the appropriate analytical environment is delivered.

  Potential breakthroughs:
  - Molecular adsorbents in practical applications to control crystallisation;
  - Enhanced low temperature process technologies for food production;
  - Intelligent labelling to control and follow production and distribution;
  - Self-assembly of barriers and capsules (moisture and oxygen migration);
  - New materials for targeted drug delivery through foods based on lipidic nanoparticles.

- **Synergy of nanofood science and industry**
  In food science, the collaboration of major academic groups with industry and food research centres is still sporadic. For future breakthroughs in nanofood science, a close collaboration between research teams and industry is essential. Entirely new metrology tools and analysis e.g., synchrotron radiation and neutron techniques would be beneficial to meet the needs of the emerging nanotechnology industry. While much progress has been made, current instrumentation and metrology are at their limits and much greater capabilities will be required, from laboratory to commercial-scale manufacturing.

- **Food processing**
  Food processing is important in the food industry and the quality of the food product is often strongly related to the control over these processes. Sensors monitor the nanoprocesses more accurately; nanotechnologies may offer further opportunities in this area:
  - High accuracy microsieves: to sieve out bacteria or yeast cells from certain beverages and pasteurise them without heating;
  - The same principle will allow fractionation of complex mixtures like milk into the different components, thus adding much value to these components;
  - The same types of devices are used in cross-flow emulsification to make monodisperse emulsions which have better characteristics than traditional or even double emulsions.

- **Product engineering**
  Food product engineering must start at the nanoscale controlling all structures of food at the nanolevel and thereby allowing engineering of the characteristics at the macrolevel.
  Key developments are:
  - Batch processing of fatty acids involves strict control of lipid crystallisation, polymorphism and crystal size;
  - Creating stable physical gels on the nanoscale;
  - Long-term gel stability as a function of time and temperature fluctuations;

- Control of the cross-linking of protein and/or polysaccharide fibrils in gels;
- Study of surfaces and interfaces between food layers (bakery products);
- Nanoencapsulation systems (adopted from the pharmaceutical industry) to protect, mask and/or deliver specific nutrients to those parts of the digestive tract where they have maximum effect.

- **Food quality assurance and safety**
  Nanotechnologies should allow to:
  - Generate instruments that can measure contamination of foodstuffs or the presence of pathogens faster, more accurately and more specifically;
  - Move food quality assurance from the lab to the production lines;
  - Enable quality to be monitored more frequently.

- **Food packaging**
  Future innovations through nanotechnological concepts are:
  - Improved barrier characteristics;
  - Coatings that reduce the microbial pressure on the food product inside;
  - Special indicators utilising nanotechnology to signal oxygen leakage in modified-atmosphere packaging;
  - Indicators providing information on the ripeness of packaged fruit;
  - Smart packaging and sensors that direct information on the quality of the product and the remaining shelf-life (combined with printable RFID electronics).

Conclusions and recommendations

Food science at the nanoscale demands a fundamental understanding of the interaction between proteins, fats and polysaccharides and of the interaction and structures at the various length scales. This task requires the development/use of advanced analytical technologies (see Fig. 5.3.28).

Analytical tools for probing nanosized/micron dimensions in food

With increasingly tighter regulations, food developments will demand clever design. As the future challenges lie in the nanometre regime, it is imperative that food science and technology should have the appropriate analytical tools available to explore the nanostructure of food. It should be clear that there will be a continuous need for top-class three-dimensional crystallographic studies of enzymes which play a crucial role in all aspects of food science as well as for the more complex and still largely lacking difficult crystallographic studies of polysaccharides, lipids and small organic molecules exhibiting polymorphism.

While electron microscopy related observations often involve highly specific sample treatments prior to 'post mortem' structure visualisation as well as the risk for radiation damage, more recently developed experimental tools, such as synchrotron radiation and neutron techniques in combination with advanced microscopy tools (STM/AFM) will improve the future progress in food sciences: i.e. x-ray and neutron reflectivity for probing surfaces and interfaces and in x-ray microtomography. Apart from the high potential to visualise structures of nanometre dimensions, there is the unique potential of synchrotron radiation and neutron techniques to observe structural changes in real-time (typically down to milliseconds), under processing conditions (heat, flow, pressure, deformation) and in a destruction-free mode.

Adequate availability of beam line access for food research is essential and a noticeably improved cooperation between the physical chemist, colloid physicists, food technologist, process food engineers and sensory experts with the large test facilities, is of vital importance. Neutron technologies could be of particular value as contrast variation will allow for the study of complex food products.

LEVEL	LENGTH SCALE	PRODUCTION LEVEL	ANALYTICAL TOOLS
Atomic	Ångstrom		Spectroscopy NMR, XRD AFM
Molecular	0.1 – 1 nm	Plant Animal	Spectroscopy NMR, XRD, WAXS Mass spectroscopy
Macromolecules	1 – 100 nm	Plant Animal Microbes Enzymes	Light scattering SANS, SAXS, WAXS Electron microscopy
Macromolecule assemblies	0.1 – 10 µm	Factories Kitchen Shelf life	SANS, SAXS Optical and electron microscopy
Products	1 µm – 10 cm	Transport Home Storage	Rheology Texture analysis

Fig. 5.3.28: Relevant length scales and the complexity of food products from production to consumption.

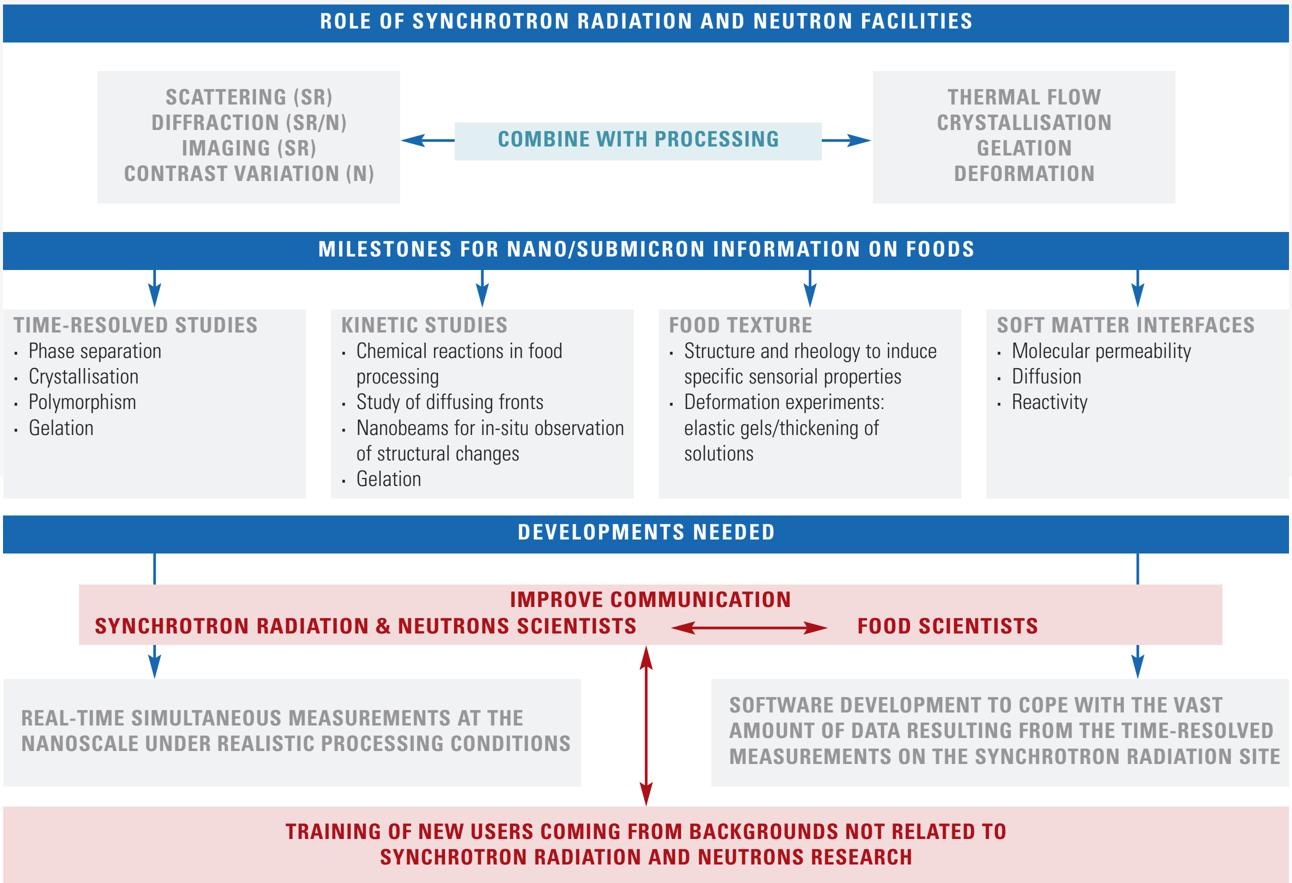


Fig. 5.3.29: Milestones for nano-/submicron information on foods.

Necessary developments at synchrotron radiation and neutron facilities

Areas which need to be addressed in order to maximise the potential of synchrotron radiation and neutrons in food studies:

- Future achievements will depend heavily on the development of new tools capable of performing real-time simultaneous measurements at the nanoscale under realistic conditions. Effective communication between synchrotron radiation and neutrons scientists and industry may lead to new analytical concepts.
- Current software is not able to cope with the vast amounts of data which result from time-resolved experiments and even from static measurements. Moreover, it would be a great advantage for on-the-run optimisation of time-resolved experiments if software was available that enabled real-time interpretation.
- Staff at facilities will need encouragement to interact and train new users from food science who will often come from backgrounds that are not related to synchrotron radiation and neutrons at all.
- Increased flux at neutron sources coupled with advances in optics development and counting devices could facilitate specific time experiments (involving contrast variation) under conditions realistically mimicking processing.
- The development of appropriate in-situ cells should reproduce high pressure, high temperature conditions and liquid flows.
- Improved resolution of x-ray tomography and imaging in the "water window" will offer new opportunities for revealing high resolution x-ray images of the complex heterogeneous structure that makes up most food materials.
- Resonant x-ray imaging may help to reveal the location of minerals and trace elements after processing, to help understand encapsulation and nutrient availability.
- Converging and multi-technique approaches must be further developed.

Milestones for food research on the nanoscale

- Time-resolved studies of dynamics in complex systems with competing interactions (phase separation, crystallisation, and gelation);
- Kinetic studies with high spatial resolution of chemical reactions, such as those occurring in food processing, in particular the study of diffusion fronts and recrystallisation within individual starch granules;
- In-situ studies by static and dynamic methods of food texture in order to account at the nanoscale for consumer's perceptions;

- Microscopic understanding of properties and organisation of the soft matter interfaces in terms of molecular permeability, diffusion and reactivity to arrive at models for the mechanism of drug release from nanosized particles.

A major challenge is to make better use of the world's capacity for food production. It will be in particular a great endeavour when food research enables raw materials from earlier parts in the food chain to be modified into foods accepted as replacements for products from later parts in the food chain. For instance, design of new foods, appreciated as meat replacement and derived from vegetable protein sources, avoids having to slaughter animals, makes meat production much more sustainable, and reduces the use of land, water consumption and waste production. To be able to rebuild the complex structural hierarchy of meat from the bottom up requires a great deal of research including advanced analytical techniques. This comprises an immense challenge for nanofood research.

Since food research is multidisciplinary, a single effort or centre cannot address all of the key challenges. It is at the nanolevel that physical changes and interactions of food biopolymers determine the designed product structure, stability and texture. Therefore, an integrated and multidisciplinary approach of key problems in the food industry is required.

In order to make progress, partnerships between food industry and nanoscientists are mandatory. Moreover, at least a "European Food Network" is needed or, even better, a "European Institute for Food Science".

Food can only be studied successfully when research is to be extended from structural and compositional studies to studies of dynamics. This work will involve time-resolved structural studies by means of small-angle scattering, diffraction, imaging and tomography. Mostly, parallel use of different techniques and the application of complicated external conditions based on pressure, flow, heat cycles, and temperature gradients will be necessary.

These conclusions should at least materialise in:

- Instrument development at large-scale facilities for multi-technique analysis, in real-time, under conditions simulating appropriate processing strategies, dedicated to food problems.
- A network of interdisciplinary researchers involved in the study of the interplay between ingredients, processing, micro- and nanostructure, food quality, nutrition and waste management.
- Enhanced cooperation between food experts from industry and academia, and scientists at the large-scale facilities.
- High priority on food research, also in the allocation of beam line access at research facilities.

5.3.8. NATURAL NANOSYSTEMS

The past decades have witnessed a renewed interest in natural materials and products in terms of research and application. This fact is primarily driven by natural products' environmentally-friendly properties as biomaterials and for their potential applications in the automotive, packaging, food, textile and pharmaceutical industries, in addition to traditional interests for instance in paper and wood. Since natural products are abundant, renewable, ultra-light-weight, inexpensive and biodegradable, they are currently used for many applications at the macroscopic levels such as electromechanical systems, insect robots, flying objects, biosensor devices, and so forth.

There is, however, an urgent need to exploit new horizons for the potential use of those natural products at the nanoscale, and therefore natural nanoscience will benefit the following:

- Improved exploitation of raw natural materials;
- Biomass valorisation;
- Optimisation of new processes for the design of precise natural macromolecular architecture;
- Transformation for applications in the framework of sustainable development;
- Development of new functionalities to be incorporated either in the new class of natural molecules or in the nanostructured ultimate state of nanomaterial fabrication;
- Hybrid sugar-synthetic (HSS) and Hybrid sugar-peptide (HSP) block copolymers:novel class of biomaterials made from natural sugars or/and synthetic or/and peptides;
- Surfaces peptides recognition properties chips;
- Explore the conditions under which the microdomain orientation and the long-range order can be controlled on 2-D and 3-D levels "defect-free" having direct consequences in nanofabrication applications;
- A wide range of interesting methodologies that can be undertaken to prepare precise architectural natural macromolecular chains including "green and click chemistry";
- Develop novel manipulation strategies based on breakthroughs that have been made in the field;
- The development and integration of nanomaterials in devices in order to fulfill specific functions in many field applications;
- Precise control over the size and the position of the nanostructures (surface density);
- Smart compartmented 3rd nanoparticles generation and surfaces with precise controlled morphology and functions for new natural nanodevices

The most cited nanonatural developments are:

- "Green" and "click" chemistry;
- Biodegradable nanoparticles;
- Surface nanosensors;
- Chips;
- Design of precise oligo- and polysaccharides offering specific functionalities.

Research needs

- Precise design of architectural natural molecules (oligo- and polysaccharides);
- Modelling of hierarchical structures that mimic mother nature;
- Possibility to monitor the dimensions by designing specific natural macromolecules such as hybrid oligosaccharides or polysaccharides-based block copolymers.
- New nanostructured biomaterials obtained from the self-assembly of natural molecules;
- Development of smart nanoparticles and surfaces decoration for drug delivery, improved diagnostics and treatments;
- Improve the host-guest biocompatibility for medical applications;
- Nanoparticles encapsulation for many application with "time-released" natural process;
- Increase the efficiency of nanostructured biodegradable materials;
- Mimic nanostructured natural assemblies in order to build stimulable biomaterials;
- Develop new and original strategies for elaborating functional polysaccharides-based nanoelectronic materials through the concept of block copolymer self-assembly and convenient manipulation of high-resolution patterns originated from their spontaneous organisation at the nanoscale level;
- Nano-insect robots, nano-flying objects, nano-electromechanical systems, nanobiosensors, and flexible electrical displays using renewable raw materials;
- More environmentally-friendly and sustainable resources such as cellulose or cellulose-based materials;
- Design and fabrication of a new class of functional polysaccharide-based materials having structures ordered down to the nanoscale, for different applications including conducting thin films (flexible electronic devices) and microelectronic devices;
- Hybrid Sugar-Peptide and Hybrid Sugar-synthetic block copolymers;
- Self-assembling of Hybrid block copolymers: nanoparticles and thin films and smart surfaces;
- Open new horizons and opportunities for block copolymer cellulose-based thin film applications (flexible electronic nanodevices) that constitute a ground-breaking development, as compared to the USA and Japan;
- To obtain to the lowest possible limit in terms of size, spacing and high density for further applications and if possible below 15 nm such as for photonic applications, since quantum confinement starts below this limit.

The research that has to be made in the synthesis of those innovative-controlled hierarchical hybrid based natural oligo- or polysaccharides/peptides could easily be extended/applied to other far-reaching fields of the industry, leading to other major impacts.

This clearly marks the beginning of a new field of „natural nanoscience" and opens up a new pathway for discoveries in nanotechnology. This strategy will have far-reaching implications in nanoscience and overall global technology research since oligosaccharides, polysaccharides and peptides are used in almost every application. Designing and controlling their architecture and self-assemblies at the nanoscale is one of the major challenges of the next decades.

Research roadmap

There is an urgent need to exploit new horizons for potential applications of those natural products at the nanoscale. Consequently, in the future it will be necessary to design and fabricate a new class of functional, natural-based materials having structures ordered down to the nanoscale. Achieving this will require a novel route consisting of developing a "versatile green approach, such as click chemistry", involving hybrid (oligo-)polysaccharide-synthetic and hybrid (oligo)-polysaccharide-peptide block copolymers. Such a new class of natural macromolecules (polysaccharides and polypeptides) should have the precise architectural molecular design that will be of great importance in developing a 2-D and 3-D level "defect-free" and high resolution nanoscale structure for different applications which can possibly solve societal challenges and be used in nanodevice fabrications.

Role of synchrotron radiation and neutrons

X-ray and neutron scattering are of great importance for the study of:

1. Elastic and dynamic properties of single molecules, nanoparticles, surfaces or bulk materials;
2. Nanostructural hierarchy;
3. Time-resolved changes in the nanostructures;
4. Rheological behaviour under shear;
5. Combined scattering and rheo-optical behaviors;
6. Block copolysaccharide self-assemblies, nanoparticles and organised thin films;
7. Dynamics at nanosurfaces;
8. Deuterium labelling of natural molecules and neutron scattering investigations for structure (SANS & USANS) and dynamics properties (Spin-Echo);
9. Decoration of nanoparticles or thin film with natural molecules;
10. Smart surfaces with precise nanostructured density of natural functionalities (oligosaccharides or polysaccharides).

Conclusions and European research strategy

The precise architectural design of new natural macro- (molecules) – oligo – or polysaccharides – combined with synthetic or peptide blocks and carrying specific functions is the new challenge for the next decades. The potential of "unmodified" natural oligo- and polysaccharide macromolecules has already been demonstrated and used for many applications (food, medicine, electronics, optics). On the other hand, controlled hierarchical design at the nanoscale level of hybrid combined sugar-synthetic or sugar-peptide block copolymer systems will be innovative and would constitute a ground-breaking development in the fabrication of nanomaterials. The development of such nanomaterials will present new opportunities for applications such as smart nanodevices, and will certainly impact societal problems in the near future.

5.4. CHEMICAL AND RELATED INDUSTRIES

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5.4.1. CHEMICAL TECHNOLOGY

Europe is a world leader in chemicals production and the chemical industry is the third most important sector in the EU, with 3 million employees in 24 000 companies, of which 96% are small and medium-sized enterprises (SMEs). However, Europe's proportion of the world trade in chemicals has dropped from 32 to 28% in the past decade, despite an increase in sales from EUR 14 billion in 1990 to EUR 42 billion in 2002 .
To sustain growth, it is mandatory that the chemical industry develops a strategic research agenda to achieve a balance between long-term technology-driven and short-term market-driven research.

Materials technology has been identified as one of several strategic areas for European innovation – having huge potential to transform the chemical industry and to create opportunities for new European companies. In addition, due to its many applications, it can have a significant impact on society and promote the development of new sustainable technologies. Developments within the field of materials technology in most cases necessitate the involvement of nanoscience and nanotechnology.

Nanotechnology will:

- Provide an understanding and control of surface phenomena that may lead to exploitation of surface functions e.g. in catalysis, electrodes, sensors, and their interfaces with gases paving the way to new and improved materials and devices.
- Allow the use of nanoparticles in composites and as coatings through an understanding of their special interfacial properties.
- Help to determine the stability and safety of new nanoparticles in dry, wet and colloid forms.

Vision for the chemical industry

- The identification of opportunities is accelerated, in close co-operation with partner industries down the value chain, leading to new and improved functionalities.
- Manufacturers will combine the benefits of traditional materials and nanomaterials to create a new generation of nanomaterial-enhanced products that can be seamlessly integrated into complex systems.
- Nanomaterials will serve as stand-alone devices, providing unprecedented functionality.
- The convergence of market demand and innovative technology development will create many opportunities for new enterprises in the materials sector, amongst which will be new high technology leaders.
- Innovation in this area will drive many innovative, high-value applications in the downstream industries.

Nanomaterials for the chemical industry

- **Nanoparticles**
  - Organic/inorganic pigments (e.g. UV-VIS-NIR pigments),
  - Inorganic functional particles (e.g. ZnO, CdS),
  - Organic functional particles (e.g. dendrimers).
- **Nanostructured materials**
  - Nanocomposites (e.g. functionalised responsive resins, ...),
  - Thermoplastics (e.g. with increased thermal conductivity, ...),
  - Foams (e.g. nanoporous foams for better insulation, ...),
  - Formulations (e.g. agricultural products, cosmetics, pharmaceuticals – with controlled delivery of actives).
- **Nanostructured surfaces**
  - Catalysis (e.g. more efficient, more selective catalysts, ...),
  - Functional coatings (e.g. anti-fog/anti-soil, ...),
  - Electronic components (e.g. printable electronics, E-paper, ...).

Application fields for these materials are given in the following figures (see Fig. 5.4.1 and Fig. 5.4.2).

MARKET OPPORTUNITIES FOR NANOMATERIALS I

Key market opportunities	Priority products/processes
Environment	· Clean water (nanofiltration, sorption, exchange) · Catalysts
Energy	· Energy conversion (photovoltaics) · Energy storage (hydrogen storage) · Batteries (high performance electrodes) · Fuel cells · Solid state lighting · Supercapacitors
Food and Agriculture	· Targeted, non-toxic biodegradable pesticides, herbicides · Time-released fertilizers and pesticides
Medical and Health	· Nanosensors · Drug delivery · Prosthetics, tissue engineering
Housing	· Multi-functional coatings (paint) · High performance insulating materials

Fig. 5.4.1: Market opportunities for nanomaterials I.

MARKET OPPORTUNITIES FOR NANOMATERIALS II

Key market opportunities	Priority products/processes
Transportation	· Nanocomposites (lighter, more durable) · Superior coatings and adhesives
Electronics and information technology	· Batteries · Nanoelectronic devices · Optical computing
Personal care	· Hair and skin care · Dental materials · Anti-ageing creams
Textiles	· Nanofibres – strong and durable · Functional fibres for soil resistance, etc.
Cross cutting	· Barrier coatings for mass transport · Self-cleaning · Antimicrobial · Electroactive and conductive polymers

Fig. 5.4.2: Market opportunities for nanomaterials II.

Knowledge-based development of nanostructured materials is needed for the following applications:

- **Membranes for separation technologies**
  Smart materials (e.g. membranes, adsorbants) have to be designed for desalination, the removal of pollutants from water, or the removal of malodours from foodstuffs. Alternatively, they can be designed in such a way that the product of a (bio-)chemical reaction is removed from the reactor, in order to shift unfavourable reaction equilibrium to the desired side, or to separate a desired (bio-)molecule from a diluted solution. All the synthetic approaches aim at a well defined nanostructured material with well-defined internal surfaces.

- **Eco-friendly antifouling coatings**
  The attachment of various forms of sea life to boats is a serious problem that is countered by the use of toxic chemicals. This could be circumvented if one could coat the vessels with a material that prevents this. This is an application where the repellent properties of biological molecules and/or a suitable nanostructuring are of importance. If one understands the mechanism of molecular recognition, one can also design a system that will repel cellular components. Anti-fouling is also an important topic for membranes, which are used for industrial separation processes.

- **Self-cleaning surfaces**
  An application could be coatings for windows so that they are cleaned by sunlight and rain, or stain-resistant coatings for clothes. Taking this one step further, one could think of self-repairing coatings, like in self-repairing paint. This relates to living systems, which are able to repair themselves using self-assembly. Can this be translated into "non-living" systems by means of artificial nanostructured surfaces resembling those of the famous Lotus leaf?

- **Smart packaging materials**
  To date, the purpose of packaging is mainly to protect the contents against dirt, contamination and/or oxidation. It would be useful to devise packaging materials that act as sensors, for example, materials that respond to the decay of meat. This would be a more reliable indicator of food quality than a general indication of shelf life on the packaging. Again, it is to be expected that new sensor systems fulfilling the above demands can be built using the concept of nanostructuring. Furthermore, it is possible to protect the food by the packaging material against UV-degradation and oxygen-attack by employing suitably nanomodified polymer films.

- **Controlled release of drugs and nutrients**
  New and better systems for the encapsulation of drugs and nutrients based on the concept of nanostructured carrier systems have to be developed. Novel concepts are needed to respond to physicochemical changes that can trigger the release of the encapsulated compound. For instance, the pH near a cancer cell is slightly lower than near healthy cells; a carrier could be made that responds to these minute pH changes and then releases the drug. Another application of materials for controlled release will be personal care products.

- **Self-organising polymers**
  These could act as templates or moulds for electronic devices, or as memories. As fabrication using the conventional top-down approach reaches its theoretical limit, bottom-up self-assembly could allow the fabrication of electronic devices in the range of 10 – 20 nm.

- **Polymer nanostructures**
  These structures could act as nanoreactors for metal nanoparticle formation, which in turn serve as markers in medical and catalytic applications.

Research targets for the next 10 years

- The design of advanced materials and composites (advanced high-strength/low-weight materials).
- The design of template nanoporous polymeric materials.
- The fundamental understanding of interfaces and nanointerfaces.
- The fundamental understanding of formulations to achieve controlled functional properties.
- The development of innovative synthetic strategies and new chemical reactions.
- The fundamental understanding of catalysis and the rational design of new catalysts.
- Improved understanding of the effect of synthesis conditions, catalyst composition and structure on the chemical and material structure and composition.
- The understanding of growth kinetics, surface grafting and modification, polymorphs, etc.

Principles to achieve these targets:

- Understand the relationship between functionality and material properties by rationales.
  The SPR-based approach is an intrinsically multidisciplinary field that implies an intimate interconnection between computational materials science, informatics, analysis and chemical synthesis.
- Integrate high throughput analysis and computational materials science.
- Accelerate the development of new material technologies through the efficient analysis of experimental data modelling, and simulation.

Implementation of research results in development and application

A key point for the transfer of nanoscience into nanotechnologies and their use will be the "implementation of nano": it is not sufficient to develop demonstrators on a small scale – but the respective nanostructures and nanofeatures must be reproducible on large scales, i.e. during scale-up and in real products (see Fig. 5.4.3). A typical example is the dispersion of nanoparticles in materials, which can be achieved either by advanced dispersion techniques or on small scales only. But it has to be noted that the desired properties, for example UV-protection combined with transparency or (increase in bioavailability), can only be achieved when the particles are formulated such that no agglomerates form and a good distribution in a matrix is achieved.

The knowledge about this formulation step is as important for the development of nanobased products as the nanosized ingredients themselves. Apart from the fundamental work on providing new nanostructures and new paths for making them, in the future, much effort will have to be invested in process design.

A fact which makes generalised and short statements about roadmaps and timelines in the field of nanomaterials extremely difficult is the fragmentation of the application areas (see Fig. 5.4.5). See section 5.3.2 for more information concerning medical applications and section 5.2 concerning nanotechnology in the semiconductor industry. To illustrate this, we mention here the miniaturisation to the nanoscale of microchip development on the one hand and on the other hand, new nanostructured and addressable drugs to fight cancer. It is evident that the only common aspect between both approaches is the length scale of ca. 50 nm of the structures involved. For an attempt to provide a rather complete survey of the various fields we refer to recent studies.

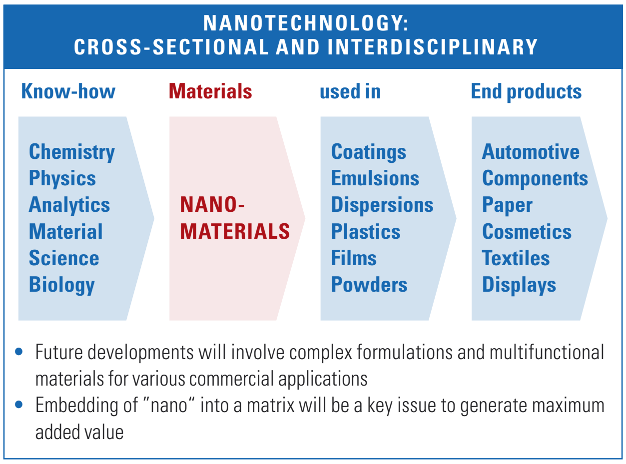


Fig. 5.4.3: Nanotechnology: Cross-sectional and interdisciplinary.

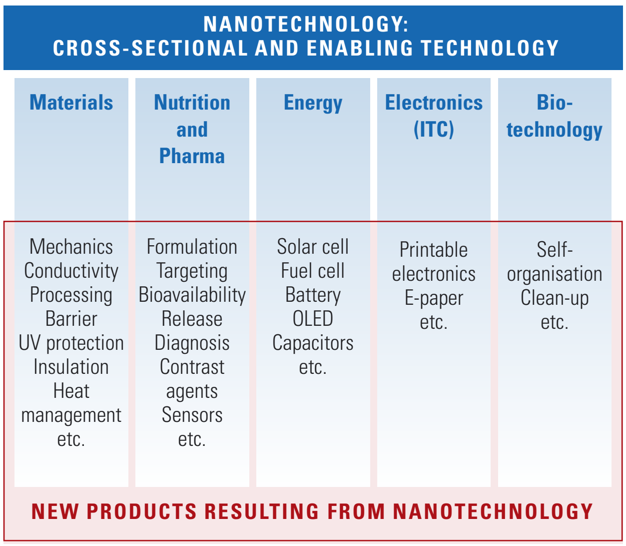


Fig. 5.4.4: Nanotechnology: Cross sectional and enabling technology.

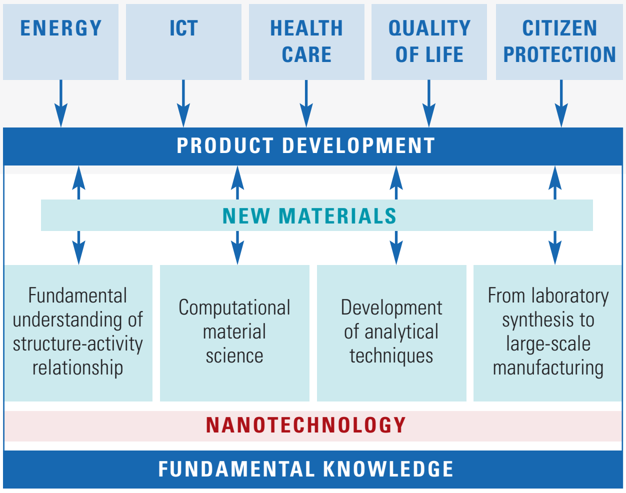


Fig. 5.4.5: Development of nanomaterials.

European technology platform for sustainable chemisty

- The vision is that accelerated identification of opportunities, in close cooperation with partner industries down the value chain, will lead to new and improved functionalities;
- Manufacturers will combine the benefits of traditional materials and nanomaterials to create a new generation of nanomaterial-enhanced products that can be seamlessly integrated into complex systems;
- In some instances, nanomaterials will serve as stand-alone devices, providing unprecedented functionality;
- The convergence of market demand and innovative technology development will create many opportunities for new enterprises in the materials sector, amongst which will be new high technology leaders;
- Moreover, innovation in this area will drive many innovative, high-value applications in the downstream industries.

The largest barrier to rational design and controlled synthesis of nanomaterials with predefined properties is the lack of fundamental understanding of thermodynamic, kinetic and quantum processes at the nanoscale. Today, the principles of self-assembly are not well understood nor do we have the ability to bridge length scales from nano- to micro- to macro. This lack of basic scientific knowledge regarding the physics and chemistry of the nanoscale significantly limits the ability to predict a priori structural properties and processing relationships. Profitable research will result in the development of kinetic and thermodynamic rules for synthesis and assembly which can be applied to the rational design of nanomaterials at commercial scales (including hierarchical nanomaterials) from first principles (see Fig. 5.4.5).

Future role of synchrotron radiation and neutron facilities

For an in-depth understanding of nanomaterials functions, it is mandatory to get a microscopic insight into the properties of the individual nanocomponents as well as understand the structure-property relation of the macroscopic system. Therefore a correlation between the spatial organisation at the nanoscale and fundamental property information (e.g. mechanical, chemical, thermal, etc.) needs to be discerned by non-destructive analytical tools.

For industrial processes, several analytical technologies dedicated to the analysis of nanomaterials are required. The advanced in-situ and non-destructive analytical tools provided by modern synchrotron radiation and neutron facilities are and will in future become even more essential for the high precision characterisation of nanomaterials for the chemical industry. These facilities open up the possibility of new characterisation techniques such as, e.g., microfocus investigations, microscopy and tomography with high spatial resolution, coupled with spectroscopic techniques.

Furthermore, it is expected that advanced, multi-probe tools will be available at the European advanced radiation sources to accurately measure the critical properties on the nanoscale and provide real-time characterisation of one-, two-, and three-dimensional nanostructures, including multiple ensemble averages and number and type of defects. Special tools are to be developed to allow fixation and manipulation of nanostructures under well-controlled environmental conditions.

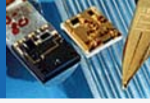
It is thus necessary to provide:

- Dedicated quick-access beam lines for the characterisation of nanomaterials in diffraction, spectroscopy, microscopy and tomography modes;
- Synchrotron radiation beam line with micro- and submicro-focus and scanning options;
- Standardised beam lines for impurity analysis;
- Robotics beam lines for nanomaterials characterisation for remote operation via internet or the grid.

The importance of synchrotron radiation and neutrons for the future research on nanomaterials in the chemical industry

Topics for future research	Why synchrotron radiation and neutrons ?
• Functional materials (soft matter, hard matter) with tailored properties based on nanostructuring, incl. thin films and surface coatings, drug implant technologies and medical prosthetics • Computer simulation of materials properties and processes including advanced processing, manufacturing systems, high-throughput experimentation, and prediction of product properties • Formulations (i.e. multi-component soft matter systems), e.g. emulsions, dispersions, formulated actives (agro, pharma, etc.)	• Unravelling (nano-) structure-property relationships by advanced and combined techniques • Understanding formation of nanostructures (phase separation, crystallisation, etc.) with high time-resolution • High-throughput experimentation with synchrotron radiation and neutrons • Unravelling (nano-) structure-property relationships by combining simulation with advanced data acquisition • Unravelling (nano-)structure-property relationships with, e.g., labelling techniques (with neutron scattering) to achieve stability, activity, ... • Understanding and control of formation and tailoring of nanoparticles by extreme resolution on time- and length scales

Fig. 5.4.6: Importance of synchrotron radiation and neutrons for the future research on nanomaterials in the chemical industry.



5.4.2. OIL AND PETROCHEMISTRY

Hydrocarbons are the major energy source of today's economy. In the petroleum industry, many practical problems ranging from the oil production in oil wells, the transport of oil from well to storage and refineries, the later use of oil products in combustion engines, etc. are all potentially better controlled by employing nanomaterials and nanoscopic self-assembling soft matter materials. This requires better knowledge of the basic microscopic mechanisms determining the behaviour of the involved materials and fluids in different environments.

Research in the oil industry addresses a vast range of problems and needs to include contributions from many disciplines. The complexity of the industry has evolved enormously over the last few decades, in response to contrasting (indeed partially contradictory) global trends towards an increase in consumption coupled with increasing concerns over impact on climate and the ultimate limitation of world resources. The increased use of high-technology solutions has become essential to identify new sources, to maintain or increase the production from existing fields, and to ensure the transformation of crude oil into an ever-cleaner energy source (see Fig. 5.4.7). It is widely believed that nanotechnology will be used to enhance the possibilities of developing unconventional and stranded oil and gas resources. Within the multi-billion dollar cost of exploration and production (E&P), a significant proportion can be attributed to the materials cost of the construction and maintenance of wells. Improved light-weight structural materials are critical for many applications, including weight reduction of offshore platforms, energy-efficient transportation vessels, and improved and better-performing drilling parts. Properties of common structural materials can be significantly enhanced by nanotechnology with the addition of engineered nanoparticles and hierarchical strategies inspired and implemented by nanosystems. It is furthermore noteworthy that high-surface area silicas, like micro-, meso, and macroporous silicas have been among the early nanomaterials explored for their exciting properties as catalysts or lubricants. Such mesoporous materials include various types of molecular structures that can be tailored to the needs of a specific application and which will see more widespread application.

The generic challenges are:

- Sustainability: increased consumption of energy, increasing concern over impact on climate, ultimate limitation of world resources, environmental considerations;
- Reservoir engineering: construction and maintenance of wells, fluid extraction and transport in porous media, exploration of reserves at increasing depth and harsh conditions;
- Transport and storage: increasingly complex mixtures of fluids (oil, water, gas and sand) in pipelines, possibility of crystallisation of aggregates, insulation of pipelines, development of emulsions for transport of heavy oils, diffusion and permeability of natural gases, hydrogen storage, sequestration (storage) of carbon dioxide (CO_2).

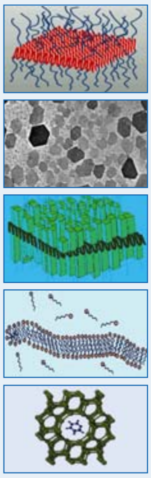
Nanomaterials will have a strong impact on the challenges pertaining to exploration, reservoir engineering and transport, and the following section provides a brief, non-exhaustive overview of very practical aspects of petrochemistry and petroengineering where neutron and synchrotron radiation should make a direct impact on research and development activities. Further fundamental research areas such as catalysis, synthesis of novel products and hydrogen-based energy systems are covered elsewhere in this volume. Advanced characterisation techniques based on neutron and synchrotron radiation technologies must play a more significant role in the petrochemical industry. The opportunities for further nanocatalysis research at large-scale facilities are significant and complement existing sophisticated laboratories by the ability to study materials in-situ in harsh or extreme environments.

OIL FIELD RELATED

Application of nanostructured fluids
- Drilling fluids
- Cementing fluids
- Water control fluids
- Sand consolidation fluids
- EOR reservoir sweep fluids

Application of nanostructured materials
- Drilling equipment (well bore)
- Light-weight construction
- Corrosion protection (coatings)

Application of nanostructured self-assembling additives for flow and crystallisation control
Wax crystallisation
Asphaltene aggregation
Clathrates in gas pipelines



PETROCHEMICAL INDUSTRY AND PRODUCTS

Catalysts in petrochemical plants
- Transport of products
- Nanostructured morphology and active sites
- Reaction kinetics and intermediate products
- Molecular sieves

Additives
- Fuel additives as flow improvers
- Viscosity modifies in motor oils

Fig. 5.4.7: Nanomaterials in the oil and petrochemical industry.

Future needs for nanomaterials research and the role of synchrotron radiation and neutrons (Fig. 5.4.8 and Fig. 5.4.9)

Nanomaterials for oil winning and recovery

(a) Exploration and reservoir engineering

Prediction of the likely target areas where to search for crude oil is greatly improved by the study of the geochemical history of an area. Laboratory techniques, such as optical and electron microscopy and x-ray and neutron diffraction, provide the bulk of the information needed. Reservoirs of hydrates of natural gas may represent an enormous untapped reserve for the future*. Hydrates are also an important topic in the transport of oil. Identification of hydrate reserves by seismic exploration relies on knowledge of the response of these solids to acoustic waves, i.e. their mechanical properties.

In high-temperature/high-pressure conditions, old electrical sensors and other measuring tools are often not reliable. In the future, nanosensors will become increasingly attractive tools for probing properties deep in the reservoir, owing to significant alterations in their optical, magnetic, and electrical properties (in comparison to their bulk analogues). This implies that nanosensors will allow to unravel the complex nature of the rock/fluid interactions and their effects on multiphase flow, as well as providing the ability to design a suitable exploitation plan for the asset.

Research potential for synchrotron radiation and neutrons

- Inelastic neutron/x-ray scattering to interrogate the vibration response of hydrates as a function of the structure;
- In-situ diffraction to determine the conditions for formation and preservation of hydrate structures in harsh environments (e.g. at pressure and low temperatures) for identification of promising areas for exploration;
- Systematic in-situ x-ray and neutron investigations of the hydrate structures and phase changes under various environmental conditions (temperature, pressure).

(b) Fluid flow in porous rocks

At present, the oil recovery factor from oil wells is between 30 to 40%. Given the oil shortages of today, an increase of the recovery factor to 60 – 70% would be a major breakthrough and would ease the world energy supply–demand balance significantly. To reach this goal, an improved understanding of the oil recovery process out of porous rock is critical. Understanding the behaviour of complex liquids in porous media is a particular challenge. By complex liquids here are meant self-assembling, multi-component systems of crude oil and water or corrosive CO_2/H_2S mixed with polymers, surfactants, etc., whose characteristic length scales are frequently identical to those of the porous materials. Such complex liquids in porous media are essential in oil production, where water comes up against petroliferous rocks. The coincidence of the characteristic length scales in the liquid and the geometric constraints from the pores has a profound influence on the phase behaviour and transport properties of the complex (nano-) liquid. Coupling the sensoring capabilities of nanomaterials (temperature, chemical composition) with the use of marking for imaging application has enhanced the understanding of fluid behaviour. Additionally, use of tailored surfactants is likely to improve the oil recovery rate.

Research potential for synchrotron radiation and neutrons

Prediction of the behaviour of crude oil/water/surfactant or polymer/surfactant systems in microenvironments based on a scientific understanding to enhance effective control of oil recovery processes; For future breakthroughs in this field, it is mandatory to carry out systematic microtomography using neutron and synchrotron radiation to provide unambiguous 3-D information of the structural properties and flow distribution of oil and water in oil-wet and water-wet matrices. Future joint efforts combining neutron and synchrotron radiation with large-scale computer simulation could be a very promising approach.

The suitability of the length- and timescales which are accessed by advanced diffraction techniques allows the microscopic exploration of macroscopic properties, i.e.:

- The conformation and aggregation of the ingredients of complex fluids;
- Their diffusion in the embedding medium, e.g. porous structures;
- The dynamic visualisation of fluid flow on the submicron scale.

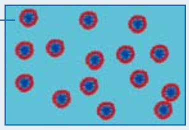
(c) Drilling and drilling fluids

Future oil discoveries are likely to involve drilling at depths of several kilometres, implying conditions of high temperature and high pressure (in an increasingly corrosive environment) that have rarely been explored up to now. Drilling operations require the development of components and new materials capable of withstanding extreme conditions. Nanocrystalline substances can contribute to harder, more wear-resistant and more durable drilling equipment, and thus reduce the cost of maintenance, repair and avoid well bore failure or loss of containment at the surface. The drilling process itself requires materials which can perform in extraordinary conditions (forces and environment) as well as special drilling fluids with very unusual viscoelastic properties such as very high shear thinning. Typical drilling fluids are mixtures of water, oil, clay, surfactants, and a high density oxide to control density. Such drilling fluids are pumped down the drill pipe to lubricate and cool the drilling bit and to carry cuttings to the surface. At the same time their hydrostatic head provides an important stabilising force against collapse of the surrounding rock. They are highly sophisticated complex fluids that are required to have tailored rheologic responses that allow for easy flow under high-to-moderate shear and gel formation when shear ceases, thus suspending the rock fragments within the borehole during change of operations when pump-

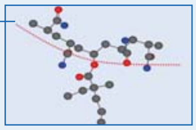
* or, alternatively, a major threat to global climate change, as methane is an important greenhouse gas (destabilisation by global warming of the world's hydrate reserves followed by further runaway warming due to methane release is a nightmare scenario envisaged by some).

QUALITATIVE INCREASE OF EFFICIENCY IN OIL RECOVERY

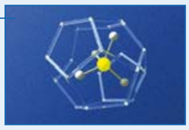
Multicomponent systems in porous media
The role of:
- Surfaces
- Self-assembling and confinement
- Phase behaviour
- Transport properties
- Inhibitors for shale swelling



Smart responsive materials
- Change of physical properties by external process triggers
- Thermo-associative polymers
- Shear induced gels for blocking of fractures



Crystallisation control
- Inhibitors for wax crystallisation
- Asphaltene aggregation
- Clathrate formation
- Cement hydration retardation



Rational design of catalyst for special chemical reactions
In-situ observation of:
- Kinetics
- Intermediate species
- Transport processes
- Active sites and there morphologies

Smart additives for functional fluids
- Self-assembling flow improvers
- Rheology control by external triggers
- Self-adapting viscosity improvers

Fig. 5.4.8: Research goals for nanomaterials research and development.

RESEARCH OPPORTUNITIES FOR SYNCHROTRON RADIATION AND NEUTRONS IN THE STUDY OF HYDROCARBONS	QUALITATIVE INCREASE OF EFFICIENCY IN OIL RECOVERY THROUGH	IMPROVEMENT OF CHEMICAL PLANTS AND PRODUCTS THROUGH
Complex fluids in porous media Structural aspects: small angle scattering, reflectometry · Self-assembly of key compounds · Adsorption, wetting, de-wetting of surfaces · Molecular response to external fields · Phase behaviour	**Multi-component systems in porous media** The role of: · Surfaces · Self-assembling and confinement · Phase behaviour · Transport properties · Inhibitors for shale swelling	**Rational design of catalysts for special chemical reactions** In-situ observation of: · Kinetics · Intermediate species · Transport processes · Active sites and their morphologies
Catalytic processes · Identification of active sites by powder diffraction · In-situ transport processes of hydrocarbons by high resolution spectroscopy · Intermediate states, reaction kinetics by high frequency spectroscopy and fast diffraction · Surface processes by reflectometry	**Tougher light-weight materials** · Cheaper oil rig construction and maintenance · Drilling equipment for harsh environments · Reduced cost of transport and risk on non-containment	**Smart additives for functional fluids** · Self-assembling flow improvers · Rheology control by external triggers · Self-adapting viscosity improvers
In-situ · Self-assembling flow improvers · Rheology control by external triggers · Self-adapting viscosity improvers · Simulated service conditions · Extreme conditions (e.g. pressure)	**Smart responsive materials** · Change of physical properties by external process · Thermo-associative polymers · Shear-induced gels for the blocking of fractures	
Visualisation · Fluids in porous media · Molecular rheology · Shear flow	**Crystallisation control** · Inhibitors for wax crystallisation · Asphaltene aggregation · Clathrate formation · Cement hydration retardation	
Dynamics · Transport processes · Molecular rheology · Shear flow		
Crystallisation control (Small Angle) · View of molecular aspects · Role of associative polymers · Molecular response to external triggers		

Fig. 5.4.9: Improvements to be expected from the introduction of nanomaterials and nanotechnology.

ing is stopped. Key to this rheologic control are hydrophobic organoclays, which are treated with cationic surfactants to compatibilise the hydrophilic core with the surrounding oil. Although these materials are widely used, the nature of the resulting gel-like structures and the complex interactions which drive their formation are not yet well understood. Additionally, special cements are already in use to reinforce the well walls and to seal them against water intrusion. Under the extreme conditions encountered and given the long exploitation times required, cement ageing is a key problem.

Research potential for synchrotron radiation and neutrons

- Characterisation and development of nanostructured materials in harsh environments;
- Understanding of complex fluids over a wide size range and under a variety of shear conditions from zero to moderate shear;
- Rheology and the structure of organoclay suspensions using SANS;
- Wide-angle x-ray scattering and optical microscopy for identification of multiple length scales and the relation between dynamic moduli, fractal dimensions of clay aggregates and volume fraction;
- Understanding of corrosion and deformation mechanisms under extreme conditions in-situ XRD and topography to determine the factors limiting materials performance;
- Basic understanding of mechanical properties of novel materials;
- Systematic (multi-technique) studies using neutron and synchrotron radiation to unravel corrosion and deformation mechanisms under extreme conditions.

(d) Oil well permeability

The oil production capability is strongly limited by low reservoir permeability either natural or caused by damage due to drilling operations. To enhance permeability, the technique of hydraulic fracturing is used with the goal to create high permeability zones to recover more oil. Specially engineered fluids are pumped at high pressure and rate into the reservoir, causing fractures to open. The fracture then extends away from the well bore and needs to be kept open by materials such as grains or sand, which are added to the treatment fluid. The complex fluids contain rod-like micelles, which have a strong impact on the viscosity of the fluid. Several physical phenomena control the behaviour of fluids in porous media. Their flow will be strongly impacted, if the pore size and the micellar size are comparable. The viscosity of the fluid also depends strongly on the phase – ordered phases, such as nematic phases lower the viscosity significantly. Flow ordering, confinement and surface templating will all influence the behaviour of these complex fluids.

Research potential for synchrotron radiation and neutrons

In-situ neutron experiments are carried out to provide an understanding of the role of:

- Confinement on liquid crystalline ordering and rheology;
- Stress, surfactant adsorption and the chemical potential in tight porous media.

More systematic and sustainable structural studies exploiting the in-situ potential of neutrons and synchrotron radiation need to be done by varying the following:

- Pore size;
- Surfactant type;
- Surface conditions;
- Shear rate.

(e) Flow assurance and transport

Given the depletion of land-based oil reserves, new production will come from off-shore deep sea fields. Flow assurance in the associated extended pipelines is crucial to the economics of such off-shore platforms. Major problems relate to paraffin or wax deposition, with the associated gelation, and to blockage as a consequence of gas hydrate formation. Flow assurance needs to control paraffin wax deposition which could be remedied by self-assembling polymeric nanostructures acting as nucleators for wax crystallisation. Due to their huge numbers, they inhibit the growth of larger crystals. Similarly, it is important to control gas hydrate crystals, which may lead to blockage of gas pipelines. Again, polymeric additives could be a solution but the mechanisms are unknown. Emulsion transport of heavy oils has been proposed as an option to decrease transport costs.

Research potential for synchrotron radiation and neutrons

- Formation and (dynamic) stability of these emulsions, as well as procedures to break up the emulsions after delivery, need to be studied both by rheological methodologies and by time-resolved small angle scattering;
- Deciphering complex fluids;
- Behaviour of self-assembling additives;
- Studying dynamic processes;
- Small angle scattering in particular can give information on the size and form of aggregates;
- SAXS using the high intensities and rapid acquisition times available with synchrotron radiation can help establish the kinetics of the process;
- All of the aforementioned research activities must be pursued in a more coordinated and systematic way;
- By the variation of contrast between the structural units or molecular groups including e.g. the embedding porous media, the components of complex systems can be studied selectively by deuteration;
- Advanced analytical techniques based on neutrons and synchrotron radiation must further the development of nanomaterials which lead to more light-weight, rugged materials that reduce weight requirements on offshore platforms, and more reliable and energy efficient transportation vessels.

Nanomaterials in petrotechnology

(a) Elemental analysis

Crude oil is a complex mixture of many hydrocarbons, and it is the detailed local environment of the carbon atoms that determine the reactivity of these organic compounds. Gas chromatography and mass spectroscopy are therefore again the main techniques here. One opportunity for element specific synchrotron radiation techniques is the study of the hetero-elements in the heavier oils, where molecular identification is difficult.

Research potential for synchrotron radiation and neutrons

- XANES has been able to provide clues as to the local coordination of S, N, Ni and V. Elimination of these elements in refining is of major environmental importance;
- Chromatography and mass spectroscopy;
- Identification of atomic and electronic structures such as the active sites in catalysts, even in-situ;
- High Sensitivity Element Analysis with sub-µm spatial resolution using focused synchrotron x-ray beams and neutrons (H distribtution);
- Standardised element analysis beam lines at synchrotron radiation and neutron facilities.

(b) Catalytic processes

In the field of supported catalysts, laboratory and synchrotron radiation methods have achieved important synergy in identifying structural and electronic characteristics. In heterogeneous catalysis, laboratory structural studies by electron microscopy and x-ray diffraction reveal information on the structure of solids containing short and long range order respectively. The supports of heterogeneous catalysts are important players in refining and petrochemistry: providing large surface areas to disperse the active phase, as well as porosity to allow reactants to diffuse to, and products to diffuse from, the active sites. To achieve large surface area, supports are typically made from poorly crystallised oxides. This lack of organisation, coupled with the fact that alumina or silica are the most common oxides, means that laboratory NMR and IR are the techniques most frequently used to obtain details of the local environment of Al and Si. Zeolites are a case apart: used both as supports and as acid catalysts in their own right, their large internal surface area as a result of long range order can easily be studied by XRD. The acid function is however again a result of local Al and Si coordination. Laboratory techniques such as NMR and IR are most often employed in these studies. The complex nature of modern catalysts, containing several phases acting either as active catalyst components or as support (or contributing to both simultaneously), can render investigation of the supported phase (often a highly divided precious metal or alloy) difficult due to superposition of information from the different structures present.

Research potential for synchrotron radiation and neutrons

- Element specific synchrotron radiation techniques such as EXAFS and anomalous XRD. The electronic information provided under vacuum in the laboratory by XPS can be enriched by in-situ studies using synchrotron radiation: both by the well-established near edge spectroscopy and by the developing high-energy XPS techniques. In addition, near edge spectroscopy can be applied to homogeneous catalysis systems to follow changes in the configuration of the metallic centre;
- High-resolution structure determination;
- The high flux and high penetration and the high space-time resolution of advanced analytical techniques using neutrons and high-energy synchrotron radiation should be fully exploited:
- To study the evolution of the system under extreme environments (e.g. pressure);
- For service conditions simulations;
- For in-situ access to catalyst behaviour (identification of transition products);
- To reveal the molecular motions leading to the viscoelastic properties of complex fluids e.g. in the microenvironment of porous materials;
- To measure larger scale dynamics which address transport processes in catalyst material.

(c) Oil additives

Lubricating oils need to be tailored to a huge range of external conditions involving additives which adopt themselves to varying temperature, shear rates etc. Such smart additives could be self-assembling nanostructured soft matter materials which e.g. change their hydrodynamic volume upon temperature, avoid shear thinning, could change their viscoelastic properties depending on external fields etc.

Research potentials for synchrotron radiation and neutrons

- In-situ structural studies the role of confinement on liquid crystalline ordering and rheology;
- Time-resolved x-ray diffraction and imaging of the role of stress, surfactant adsorption and of the chemical potential in tight porous media;
- Combined diffraction and infrared microscopy analysis of fluid inclusions;
- X-ray/neutron trace element analysis of crude oil during migration.

(d) Wax control

The agglomeration of asphaltenes, the waxing of pipelines but also the clathrate formation and its impact on the blockade of pipes, is a major concern in oil recovery and can be controlled by additives. The assembling phenomena of additives in the control of crystallisation are relatively poorly understood. Normal alkanes crystallise at lower temperatures and tend to plug filters in cars or inhibit flow in pipelines. Since the crystal growth is sensitive to impurities, the size and the shape of the wax crystals may be modified by additives. Such additives are typically polymers, which, so far, have been chosen largely by trial and error. They function through the self-assembling capacity of polymers.

Research potential for synchrotron radiation and neutrons

- Understanding the interplay between the polymer aggregates and the wax crystallisation;
- Design of polymeric templates acting as nucleator for wax crystallisation to qualitatively increase their efficiency and make fuels compatible over a large range of environmental conditions;
- Systematic x-ray and neutron studies of the microscopic phenomena leading to the agglomeration of asphaltenes and clathrate formation;
- Detailed x-ray and neutron investigations to unravel the role of additives.

(e) Energy-storage

For the coming generations, transport and storage of hydrogen may be as great, if not a greater problem than that of organic fuels, and there are strong arguments towards hydrogen-based energy storage. Again, low permeability compounds need to be developed for pipes and reservoirs. New light-weight materials need to be developed to contain hydrogen in a compact manner if its use for transport is to be generalised. The most promising systems are low molecular weight reversible hydrides.

Research potential for synchrotron radiation and neutrons

- Understanding hydride formation and kinetics, storage with a wide range of neutron and synchrotron characterisation techniques (EXAFS, SAXS/SANS, PX);
- In-situ investigation of resulting phase changes due to "charging – discharging" cycles.

(f) CO_2 sequestration

Reducing the environmental impact of industrial activity is a major challenge to modern society in which the petroleum industry is a key player. In addition to the production of cleaner, low carbon fuels, capturing the carbon dioxide produced during fuel use can reduce the impact on the atmosphere. Underground sequestering of CO_2 in depleted wells is one option which needs to be considered, but predicting the fate of the sequestered gas involves studies of gas – water – rock interactions in reservoir conditions. The same is true for prediction of the behaviour of the cement seals used to close wells used to inject the gases.

Research potential for synchrotron radiation and neutrons

- Laboratory-based x-ray end microscopy studies of phase transitions and precipitation should be complemented by in-situ diffraction and tomography studies using synchrotron radiation and neutrons.

(g) Environmental aspects

Pollution by chemicals or gases is a most challenging aspect of petroleum production. One of the future visions is that nanomaterials will render the petrochemical industry considerably greener. Filters and particles are now being developed with a nanostructure that allows removing volatile organic compounds from oil vapour and mercury from soil and water. Filters and membranes designed with nanoscale precision provide full control over what flows through.

Research potential for synchrotron radiation and neutrons

- In-situ real-time studies using synchrotron radiation and neutrons to explore structural changes in membranes and filtering nanostructures during operation.

Summary and recommendations

As readily accessible reserves become depleted, the oil industry faces increasing technical challenges, which lead to increased costs and limit the operating envelope of drilling and production technologies. This represents a significant market opportunity for nanomaterial-based solutions, as very few nanomaterials and nanotechnologies have yet to enter the range of exploration and production technology. Advanced in-situ techniques based on neutrons and synchrotron radiation carry a unique analytical potential which must be exploited in the creation of the knowledge-base needed to solve important research problems in the petroleum industry and in energy technology in general.

Future role of neutron and synchrotron radiation facilities

In order to unravel the behaviour of nanomaterials, hydrocarbons, fluid additives and related materials in different, even harsh environments, the advanced analytical technology built up at modern neutron and synchrotron radiation facilities will play a key role in the future.

Such complex materials and liquids are multi-component, multi-scale systems of metallics, ceramics, polymers, colloids, micelles and surfactants whose characteristic length scales are frequently identical to those of the porous materials. The ability to predict the behaviour of oil/surfactant, polymer/surfactant, inorganic clays/surfactants, etc. systems in microenvironments based on a scientific understanding would enable effective control of many of the processes at the oil well including possibly new routes in tertiary oil recovery. Neutron techniques are unique in this field, since even in a crowded environment or porous media the components of interest can be targeted directly by contrast variation. Furthermore, the development of novel nanostructured catalysts will increase the efficiency of oil-refinement processes. Studies of entrapment and molecular transport within porous structures are relevant to a wide range of areas from the recovery of residual oil in oil wells, to catalysis. Likewise, new tougher and light-weight nanostructured materials promise significant cost savings.

The key advantages of the analytical techniques at neutron and synchrotron radiation facilities are:

- Characterisation techniques at all relevant length- /timescales;
- The ability to perform in-situ and real-time investigations in harsh environments.

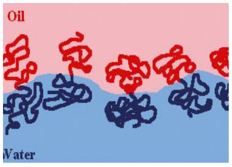
Special potential of neutron techniques

The future investigations of hydrocarbons will strongly benefit from neutron scattering (see Fig. 5.4.10):

- The length- and timescales accessed by neutron small angle scattering (SANS) and neutron spin echo (NSE) allow the exploration of large-scale properties, including the conformation and aggregation

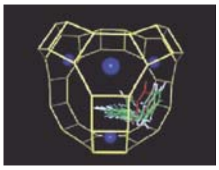
Complex fluids in porous media
Structural aspects: Small angle scattering (SANS), Reflectometry
- Self-assembly of key compounds
- Adsorption, wetting, dewetting of surfaces
- Molecular response to external fields
- Phase behaviour

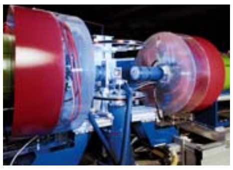
Catalytic processes
- Identification of active sites by powder diffraction
- In-situ transport processes of hydrocarbons by high resolution spectroscopy
- Intermediate states, reaction kinetics by high frequency spectroscopy and fast diffraction
- Surface processes by reflectometry



Crystallisation control (SANS)
- View of molecular aspects
- Role of associative polymers

Molecular response to external triggers (SANS)





Dynamics by neutron spin echo
- Transport processes
- Molecular rheology
- Shear flow

In-situ information of smart additives in functional fluids
- Self-assembling additives information by SANS
  - Fuels
  - Lubricants
- Responsive fluids
- Additive response to external triggers

Fig. 5.4.10: The role of neutrons in the oil-, gas-, and petrochemical industry.

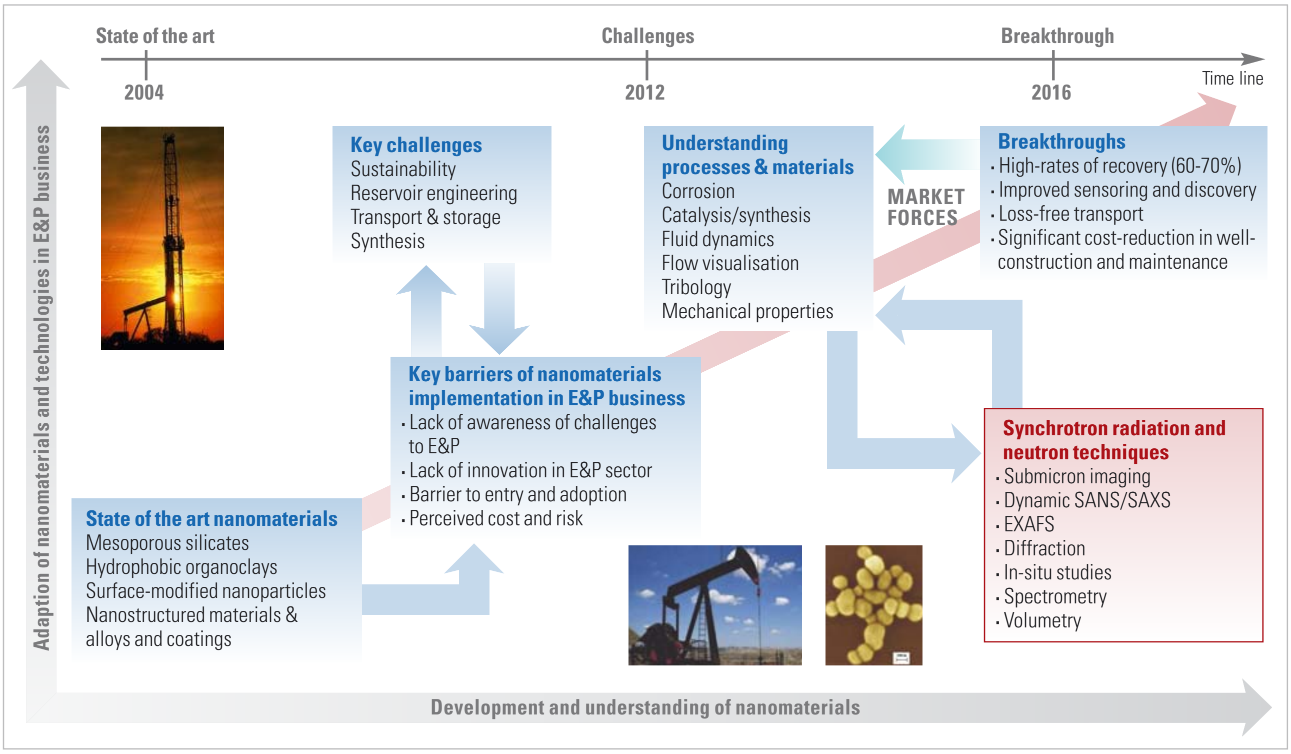


Fig. 5.4.11: Roadmap for nanomaterials in the oil- and petrochemical industry.

of the ingredients of complex fluids, and their diffusion in the embedding medium in particular porous structures. Neutron powder diffraction is a powerful tool for the identification of atomic structures (as the active sites in catalysts).

- By the contrast variation between the structural units or molecular groups including the embedding porous media, the components of complex systems can be studied selectively. In particular, the large contrast achieved by isotope substitution of hydrogen – one of the main components of hydrocarbons – by deuterium constitutes the most powerful tool for deciphering complex fluids, self-assembling additives and dynamic processes in these materials.

- The high penetration of neutrons allows the destruction-free study of the influence of external fields e.g. shear or pressure and the evolution of the system under extreme environments. It also facilitates an in-situ access to catalysts.

- The space-time resolution of neutron spectroscopy reveals the molecular motions leading to the viscoelastic properties of complex fluids e.g. in the microenvironment of porous materials. In the case of catalysts, the vibrational patterns may be used as fingerprints for the identification of intermediate products. The observation of larger scale dynamics addresses transport processes in catalyst materials.

Recommendations for large-scale facilities (Fig. 5.4.11)
The following recommendations should be implemented by the large-scale facilities in order to comply with the scientist's and industrialist's needs at the available facilities:

- Increased collaboration with companies involved in nanomaterials and nanotechnology and liaising with oil exploration and production businesses to foster R&D activities;

- A step-increase in development of dedicated facilities to provide a platform for petrochemical R&D activities, ranging from improved/complex instrumentation to complementary facilities (e.g. deuteration labs) and alignment of R&D in research strategies;

- Improved computer modelling & simulations capabilities providing complementary research output.

5.4.3. CATALYSTS

The catalytic process provides a means of changing the rates at which chemical bonds are formed and broken, of steering the yields of chemical reactions towards pathways that lead to the increased formation of desirable products and reducing the amounts of by-products (see Fig. 5.4.12). Catalysis can thus be used to obtain and govern the composition, properties, and morphologies of materials, especially the meta-stable materials that cannot survive the rigorous conditions of un-catalysed synthesis. Catalysis is therefore a key concept in realising chemical conversions in a sustainable way.

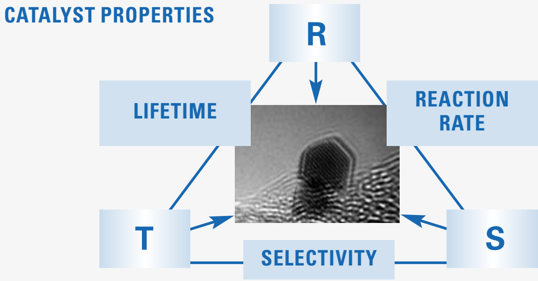


Fig. 5.4.12: The three principal factors governing the performance of a catalyst are: i) Activity (R) which is the reaction rate, ii) selectivity (S) which is the ability to produce the desired products over by-products, and iii) the lifetime (T) or stability of the catalyst material.

Regarding the relevance of the multitude of both new and well-established catalytic processes worldwide and the production volumes of value-added products, improvements of performance and yield are of paramount economic impact, even if only in the few percent regime. These improvements can allow for substantial savings in costs as well as resources. In addition, it will prove essential to improve the understanding of catalyst deactivation processes by coking, poisoning, degradation and, hence, conceiving new strategies for the enhancement of lifetime, for the improvement of activity and of selectivity by tailoring and or changing composition, nanostructure and operation conditions.

Recent developments in nanoscience enable a jump in synthesis of novel catalysts using strategies such as templating, self-assembly and lithography. These advances provide unique opportunities to design and construct nanostructured catalysts with optimum activity and superior selectivity. The grand challenge for nanocatalysis will be to achieve a microscopic ("atom-by-atom") understanding of how to design catalyst structures and how to control catalytic activity and selectivity. Future science in nanocatalysts will allow the design of completely new catalysts and catalytic processes with enhanced performance, i.e. highly active, stable catalysts that provide near~100% selectivity to a desired product with minimal use of energy; These processes will allow for as yet unimagined purposes and benefits to society, in ways which remain unthinkable in today's day and age.

A central task is to work out and substantially improve adequate techniques and strategies to study industrial catalysts under realistic conditions by utilising the unique properties of neutron and synchrotron radiation techniques. Depending on the location of hydrogen-containing entities, neutron scattering can be used as a surface science or as a bulk technique to study the proton dynamics of catalysts or materials of catalytic relevance. The use of synchrotron radiation in combination with advanced in-situ equipment and flow-through reactors will allow for fast studies of working catalysts also under realistic gas pressures and temperatures. The knowledge of such unique features is still not disseminated adequately enough. GENNESYS should act as a disseminator of information between large-scale facilities, academia and industrial research.

Future roles for catalysts materials

ENERGY PRODUCTION	PROCESS IMPROVEMENT	NOVEL MATERIALS
Large-scale hydrogen production from renewable sources: · Mimic the photosynthesis · Energy efficient production with minimum CO_2 emission through photocatalytic water splitting · Semiconductor materials with the necessary quantum yield and stability under visible light **Catalytic biomass conversion (bio fuels):** · Zero-emission fuel production from bio-feed-stocks · Catalysts are challenged by impurities and diverse feedstocks compared to fossil fuels · Stability, separation and regeneration are key factors **Conversion of natural gas and coal (with CO_2 management):** · Breakthroughs are required in direct conversion of methane · Activation of methane · Gas-to-liquids (GTL) and coal-to-liquids (CTL) technology to produce clean fuels from natural gas and coal	**Reduced gas emissions:** · Clean-up of fuel and exhaust gases to improve air quality (locally) and to limit global warming · Selective catalysts that can perform at low partial pressures without significant increase in process complexity **Process intensification:** · Design completely new materials with activity and stability beyond what is possible today to reduce cost and energy consumption in process units · Multi-stage approach including process engineering, simulations and nanoscience **Desulphurisation catalysts:** · Selective catalysis of sulphur-containing species. · Activation of stable sulphur species. · More tolerant catalysts towards poisoning and deactivation	**Production of high-performance nanomaterials:** · Use catalysis in cost-efficient production of nanotubes, polymers and composites · High demand for pure products · Need to solve catalyst-product separation. · Products highly dependent on choice of catalyst **Selective chiral catalysis:** · To use catalysts to control the three-dimensional structures of products, including enantiomeric selectivity · Asymmetric catalysis with 100% selectivity. · Heterogenisation of processes through immobilisation on solid supports · Miniaturisation **Multifunctional materials:** · Structured catalyst that combines reactor and catalyst in one unit · Combine catalysts with chemical storage/looping, selective permeability and catalytic activity

Fig. 5.4.13: Future roles for catalyst materials.

Research roadmap for nanocatalyst materials

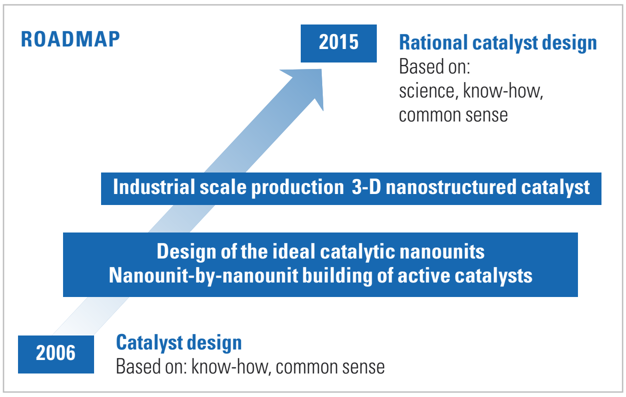


Fig. 5.4.14: Research roadmap for nanocatalyst materials.

Key challenges in the development of nanocatalytic materials

The key challenges in the development of improved catalytic materials are listed below:

Synthesis of catalytic materials (see Fig. 5.4.15.)

- "Atom-by-atom" design and manufacturing of catalyst materials based on fundamental atomic-scale understanding and tailoring the catalytic activity and selectivity;
- Identification and design of active sites in catalyst materials in order to tailor the selectivity;
- Use of catalytic reactions to synthesise new nanostructures.
- Development of new synthesis routes and in-situ control of the whole process;
- Mimic of the reaction rates and of the selectivity of enzymes.
- Use of catalysts to control the three-dimensional (3-D) structures of products, including enantiomeric selectivity;
- Screening of families of potential catalysts.

Structure/properties relation

- Establishment of firm relationships between catalyst structure, rates, and selectivity of elementary reaction steps;
- Creation of theoretical and experimental database methodologies to perform data mining with the goal of optimising the design of new catalytic systems;
- In-situ monitoring of chemical, spatial, and temporal properties of working catalysis;
- Understanding and prediction of the relation between material properties and reactivity by in-situ characterisation methods under reaction conditions;
- Understanding the non-uniformity of catalytic reactions;
- Close interactions between theoretical/computational and experimental researchers to develop advanced modelling and simulation tools that are acceptable to the entire catalysis community.

Catalyst supports

- Understanding of the thermodynamics, and kinetics of the nucleation, growth, and sintering of supported metal catalysts;
- Design of new, non-natural nanoporous and mesoporous supports for catalysis that control their chemical and physical properties and isolate catalysts in nanocages, controlling reactant access and product egress.
- Understanding the mechanisms for upscaling the catalytic properties of single nanoparticles into many kilogrammes.

- Synchrotron and neutron techniques are well-suited for the study of porosity, fractality and homogeneity;
- Neutron studies are unique in the improvement of the proton-related surface chemistry of activated carbons, carbon blacks and novel grades of carbonaceous matter used as support materials for e.g. chemical catalysts and fuel cell catalysts;
- A better understanding of redox reactions during the impregnation of support materials in catalyst manufacture is also of paramount importance. In addition, improved understanding of the effects of hydrogen-spillover and hydrogasification effects is necessary;
- A pragmatic goal is to clarify the key-properties of a "good" catalyst support (oxides, mixed oxides, carbons, membranes etc.) adequate for a certain process or technical application at the level of surface science experiments on highly dispersed matter.

Importance of nanocatalyst materials for the future of European industry

Industrial chemical plants based on catalysis accounts for 60% of current chemical products and 90% of current chemical processes. A majority of products made today are being produced with traditional methods developed during the 1950s and 1960s.

In order to keep the European process industry competitive worldwide, a technological advantage will be a prerequisite. New innovative nanocatalyst-based processes will have a strong impact on economic competitiveness and the environment. They also provide confidence that the unique catalytic properties of any single nanoparticle can be replicated into many kilogrammes of catalyst material, all of it exhibiting the same catalytic properties, for research, pharmaceutical synthesis, or industrial processes. Nanocatalyst materials are a key to future breakthroughs within a range of important industrial sectors such as the chemical- and petrochemical industry, energy technologies, pharmaceutical industry and transport industry (see Fig. 5.4.18).

Catalysts will ensure our future quality of life and the strength of our economy by:

- The reduced emissions of modern cars;
- The effective use of natural resources: raw materials and energy sources: creating alternative energy sources and new conversion technologies such as fuels cells, and devices for photocatalytic splitting of water to form hydrogen and oxygen;
- The manufacture of new materials such as polymers with tailored nano-, micro-, and macroscopic properties suited for new technological applications;
- Reducing harmful by-products in manufacturing, cleaning up the environment and preventing future pollution, dealing with the causes of global warming, protecting citizens from the release of toxic substances and infectious agents;
- The precise synthesis of molecules such as pure safe drugs and

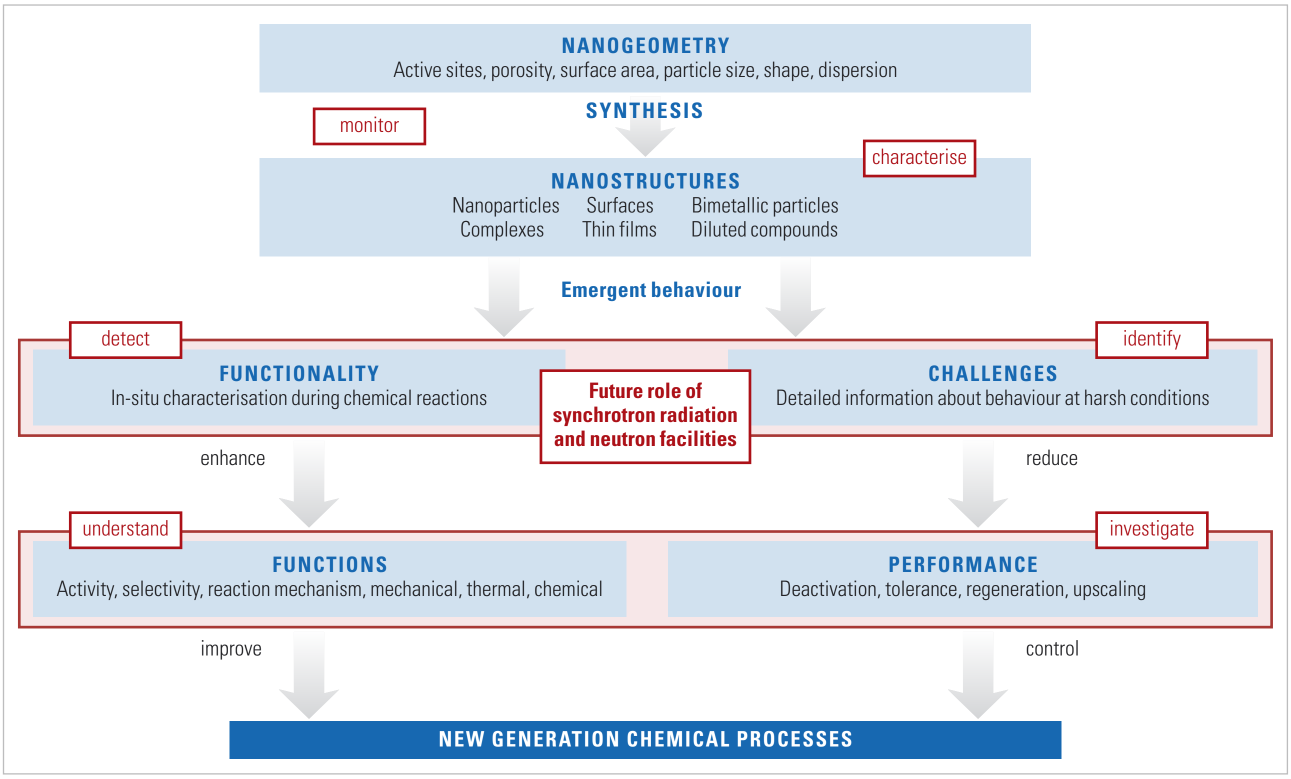


Fig. 5.4.15: Role of synchrotron radiation and neutron facilities in nanocatalyst materials research in the future.

cosmetics without toxic stereo-isomers: ref. the petroleum, chemical, and pharmaceutical industries, the reduction of pollution: smog, acidic rain;
- The improvement of product quality: production of chemicals with a minimal energy input and without environmentally damaging side products;
- Feeding the world: agriculture and fertilizer industry.

This revolution can become reality through the application of new methods for: i) synthesising and ii) characterising molecular and material systems. Opportunities to understand and predict how catalysts work at the atomic scale and the nanoscale will appear and be made possible by: i) revolutionary developments in catalyst design, synthesis, and evaluation; ii) in breakthroughs in new measurement techniques and imaging, and iii) computation.

Role of synchrotron radiation and neutron facilities

The analytical potential provided by modern synchrotron radiation and neutron facilities as well as future x-ray free electron facilities is of key importance for the further development of catalytic technologies (see Fig. 5.4.16). The main areas for the application of these advanced analytical techniques are the in the following areas:

- **Advanced in-situ structural characterisation**
  - Chemical composition, structure and morphology;
  - The ability to bind and retain molecules (adsorption);
  - The ability to chemically convert the molecules;
  - Real-time observation of the active site and how molecules are converted on a catalyst surface;
  - High temperature and pressure characterisation;
  - Structural studies of the activated state to microscopically assess the catalyst performance;
  - Exploit different scattering contrast for x-rays and neutrons to monitor the entire range of elements in the catalyst materials;
  - Unravelling structure-activity correlations and study multifunctional materials.

- **Imaging of individual catalyst nanoparticles during reaction**
  - Imaging of individual catalyst particles through nanofocusing devices;
  - Imaging of local phenomena (active sites, selective adsorption, homogeneity, sintering, poisoning).

- **Ultrafast diffraction and spectroscopy**
  - Femtosecond time-resolution from pulsed free-electron sources to study ultrafast changes and turnovers;
  - Time-resolved study of fast chemical reactions and of reaction pathways to identify intermediates and synthesis routes.

- **Dedicated facilities for catalysis studies**
  - User-friendly operation;
  - Remote control of experiments;
  - Beam lines for industrial user groups with experience on advanced, physiochemical techniques.

- **Combination of high-end computational resources and large-scale experimental facilities.**
  - New computational techniques must be developed to analyse the data from such studies and to provide a self-consistent representation of the structural and electronic features of the operating catalyst under realistic conditions;
  - High-throughput experiments for fast screening of materials;
  - Introduction of advanced characterisation methods as a tool in the simulation of process parameters and process design.

- **Key conclusions**

The main topics for research on catalyst nanomaterials in the coming years will be to:
- Develop techniques able to "measure" the active site under working conditions;
- Obtain a fundamental understanding of the reaction pathways in order to be able to rationally design nanocatalyst materials;
- Upscale advanced and precise synthesis methods to pilot plant sizes and quantities;
- Develop new multifunctional catalyst materials in order to improve and simplify chemical processes.

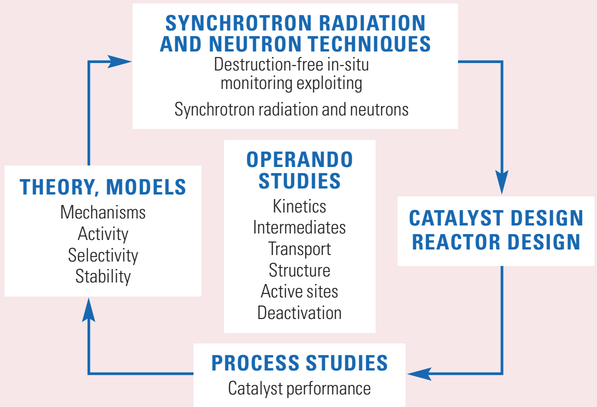


Fig. 5.4.16: The analytical potential provided by modern synchrotron radiation and neutron facilities as well as future x-ray free electron facilities is of key importance for the further development of catalytic technologies.

Key recommendation: Science Centre catalyst nanomaterials

Large-scale rational design of catalyst nanomaterials and the ability to identify and observe the active sites under working conditions has been highlighted as a key barrier for the future design of catalyst nanomaterials. Synchrotron radiation and neutrons offer unprecedented opportunities to detail the electronic and physical properties of nanostructured catalysts and to "see" these catalysts functions in a realistic environment. What remains to be established is a mechanism for exploiting these tools for the evolution of catalysis science.

Regional, national and European funding agencies, and the European Commission must positively influence the evolution of the field of catalysis:

- By articulating the importance of catalysis;
- Sponsoring workshops;
- Modernising national facilities.
- Bolstering funding for fundamental research in catalysis, and emphasising interdisciplinary Grand Challenge research,
- Creating a European Science and Technology Centre for Nanocatalysis Research.

It is of the utmost importance to create a new European Science and Technology Centre for Nanocatalyst research at a synchrotron radiation/neutron facility (see Fig. 5.4.18). The research and industry programmes could be framed in the:

- Design of new (nano-)catalyst materials based on fundamental understanding;
- Tailoring of nanoparticles and multifunctional catalysts to improve and simplify chemical processes;
- Exploration of catalytic processes;
- Performance studies under industrially relevant conditions; including the development of techniques to visualise active sites under catalyst working conditions;
- Up-scaling of advanced and precise synthesis methods.

Capabilities for the Science Centre should include:

- Set-up of multi-disciplinary research teams, bringing together expertise from a wide range of disciplines: experts in bio- and surface sciences, in nanomaterials, familiar with large test facilities, computational science and molecular modelling;
- Integration of skills across a wide range of areas: catalyst synthesis, catalyst characterisation, determination of pathways and the dynamics of elementary processes, and the theoretical methods for predicting the structure of active centres and their catalytic properties;
- Dedicated beam lines with combined diffraction and spectroscopy capabilities for in-situ characterisation of nanoparticles during chemical reactions.
- Combined structure analysis and online product analysis allowing for real-time studies of chemical reactions;

INDUSTRIAL SECTOR		RESEARCH PRIORITIES	KEY BARRIERS	Contribution from synchrotron radiation and neutrons
Energy	• Transport • Automotive • Refining	· Process intensification · Higher efficiencies · Multifunctional reactors · Sustainable feedstocks · Hydrogen · Green processes and products · Clean fuels · Miniaturisation for portable devices	· CO_2 capture · Methane slip · New feedstocks · Hydrogen storage capacity · Stable filters for diesel engines · Upscaling of novel synthesis methods	• Fast structural analysis of catalysts • Profiling catalytic materials • In-situ studies (kinetic pathways, deactivation mechanisms) • Kinetics of hydrogen storage/release
	• Solar/ photocatalysis	· Orders of magnitude higher yields · Environmental remediation · CO_2 conversion · Smart reactors · Catalytic coatings	· Kinetics · Electron/hole separation and recombination · Stability · Efficiency	• High throughput structural analysis • Local structure of solid/solid interfaces • High throughput synthesis/structural analysis of new catalysts
	• Fuel cells	· Stable, inexpensive materials · Novel materials · Tuning of the temperature window of operation	· CO tolerance · Catalyst stability · Material cost · Permeability of membranes · Miniaturisation	• Structure of electrocatalyst • Local conductivity • Local structure of solid/solid interfaces
Bulk chemicals	• Petrochemicals • Polymers • Biofeedstocks	· Structured catalytic reactors · New materials · Design and synthesis of ligands · Coatings · Minimisation of environmental impact (SO_x, NO_x, PM, CO_2) · Knowledge-based tailoring of catalyst	· Catalyst stability · Selectivity · Reliable high throughput testing/ synthesis · Good catalyst for emission · Upscaling of novel synthesis methods	• 2-D and 3-D structure • Local catalyst structure: valence, coordination, size • In-situ studies (stability, kinetics, information nanopores, clusters) • Rational development of emission abatement catalysts
Fine chemicals and pharma	• Specialties • Medicine	· Novel classes of versatile catalysts · Reduction of impact on environment · Fast structure elucidation · Microreactors	· High throughput testing/ synthesis of (multifunctional) catalysts · Time to market	• High throughput structural analysis under reaction conditions • Study realistic systems • Information on catalyst stability • New catalysts for waste reduction

Fig. 5.4.17: Spectrum of potential nanocatalysts applications in industry and needs of synchrotron and neutron facilities for breakthroughs in this highly innovative area.

- Accommodating both state-of-the-art novel experiments and standard, routine characterisation;
- High-throughput measurements for catalyst screening;
- Nano-imaging facilities;
- Access to the high-end computational resources, nanocatalyst-fabrication facilities, and characterisation instrumentation;
- Computing facilities for assisted, standardised data analysis to lower the user threshold and speed up data processing;
- Having capable scientific staff that can support and run complex apparatus on a wide range of problems;
- Education and training involving large-scale facilities, universities and industry.

This European Science Centre and Facilities provide strong intellectual, financial and European incentives for promoting catalyst science in Europe, allowing the design and execution of complex experiments and integration with theoretical efforts. Facilitating and linking the work of industry, academia, and national laboratories will drive the new developments and discoveries in catalysis that will enable Europe to regain its superiority and maintain its leads in this pivotal economic engine.

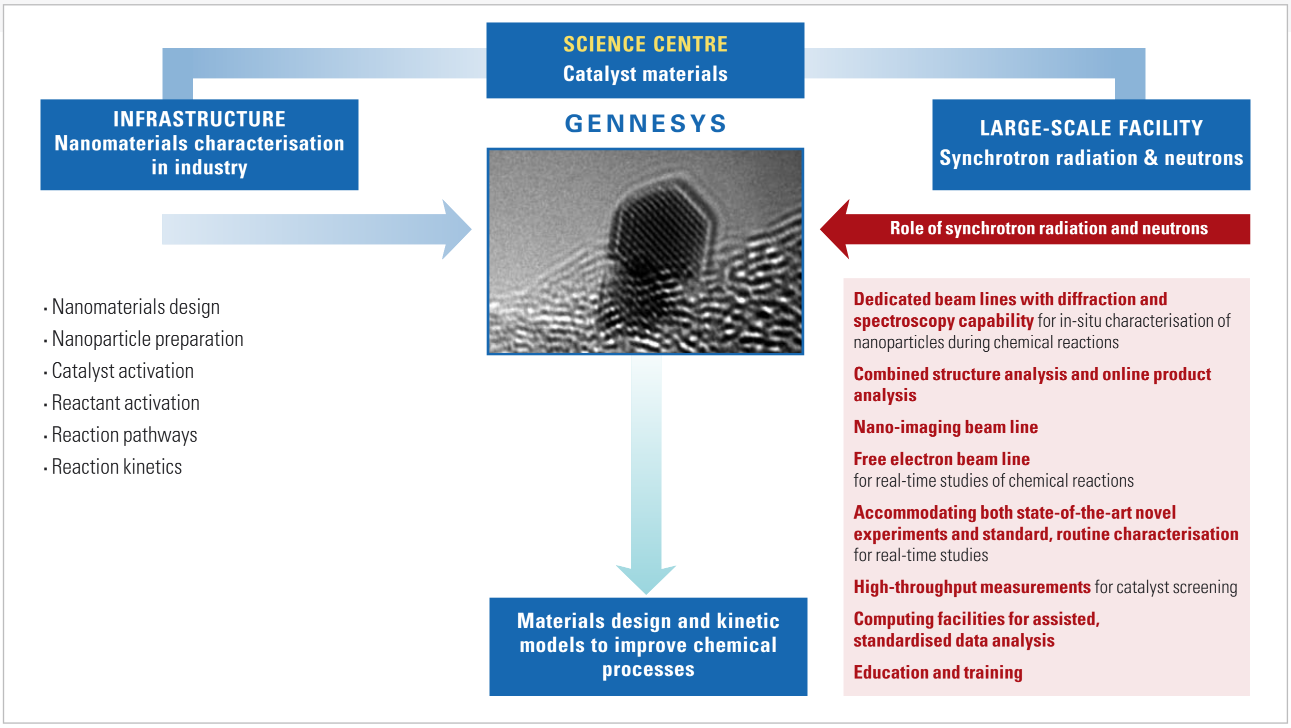


Fig. 5.4.18: Science and Technology Centre for Catalyst Nanomaterials Research installed in the vicinity of large test facilities.

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[Affiliations chapter 12]

5.5.1. NANOMATERIALS FOR NUCLEAR FISSION TECHNOLOGY

The future generation (Gen IV) of fission reactors such as Sodium-cooled Fast Reactors (SFR) or Gas-cooled Fast Reactors (GFR) requires the development of materials able to withstand high irradiation loads at high temperatures. According to the temperature range encountered in the future reactors and irradiations doses, two main concepts of nanostructured materials are considered. The first one concerns nanoreinforced steels by oxide (ODS), and the second one nanostructured composite ceramic materials (carbide ceramics). Fig. 5.5.2 gives an overview of where nanomaterials should play an important role in the future reactors.

Challenges in the development of new nanomaterials for nuclear systems

ODS (Oxide Dispersion Strengthened) ferritic/martensitic steels are promising candidates with a potential to be used at elevated temperature under severe neutron exposure environment (high burn-up fast neutron), as expected in advanced fuel cladding for Sodium-cooled Fast Reactors (SFR). Indeed, these materials present some good properties which are relevant for the nuclear environment. However, requirements of the next generation of sodium-cooled fast reactors will involve, in nominal conditions, irradiation doses >150 dpa and temperatures in the range 400°C–650°C.

ODS steels are produced by powder metallurgical methods, like mechanical alloying processes where the alloy is produced by mixing the powdered components, compacting, sintering, extruding and rolling them into the required shape (sheet, bar or tube for cladding application).

During the mechanical milling, Y_2O_3 powder (very stable oxide used for application at high temperature) can be totally dissolved in the matrix, followed by a very homogeneous nanometre scale precipitation during consolidation. In a second step, during the manufacture of tubes, bars and sheet, it is very important to control the evolution of metallurgical characteristics (for instance the grain size or the grain morphology of the material) with appropriate heat treatments and processes. In fact, the final mechanical properties are very sensitive to the fabrication route. Finally, benefits are taken from a ferritic/martensitic matrix with respect to swelling problems (free stress deformation under irradiation) and from the nanoscale dispersion of yttrium oxide precipitates, endowing these alloys with a very good creep resistance at high temperatures.

The ODS grades currently developed in the frame of the SFR or fusion contain 9 to 12% Cr. However, these alloys could show some limitations in terms of internal corrosion (oxide clad reaction) and temperature (phase transition around 800°C). Therefore, ferritic steels with 14%–18% Cr could be used up to 900°C provided that the crystallographic texture is well controlled during the fabrication process. Although irradiation data are scarce, the bcc crystalline structure should present an excellent resistance to swelling.

The main in-service issues, in the low temperature range, are threefold:

i) The effect of the materials unmixing on the mechanical properties;
ii) In the high operating temperature domain, the required stability of the Oxide Dispersion to maintain the improved creep resistance;

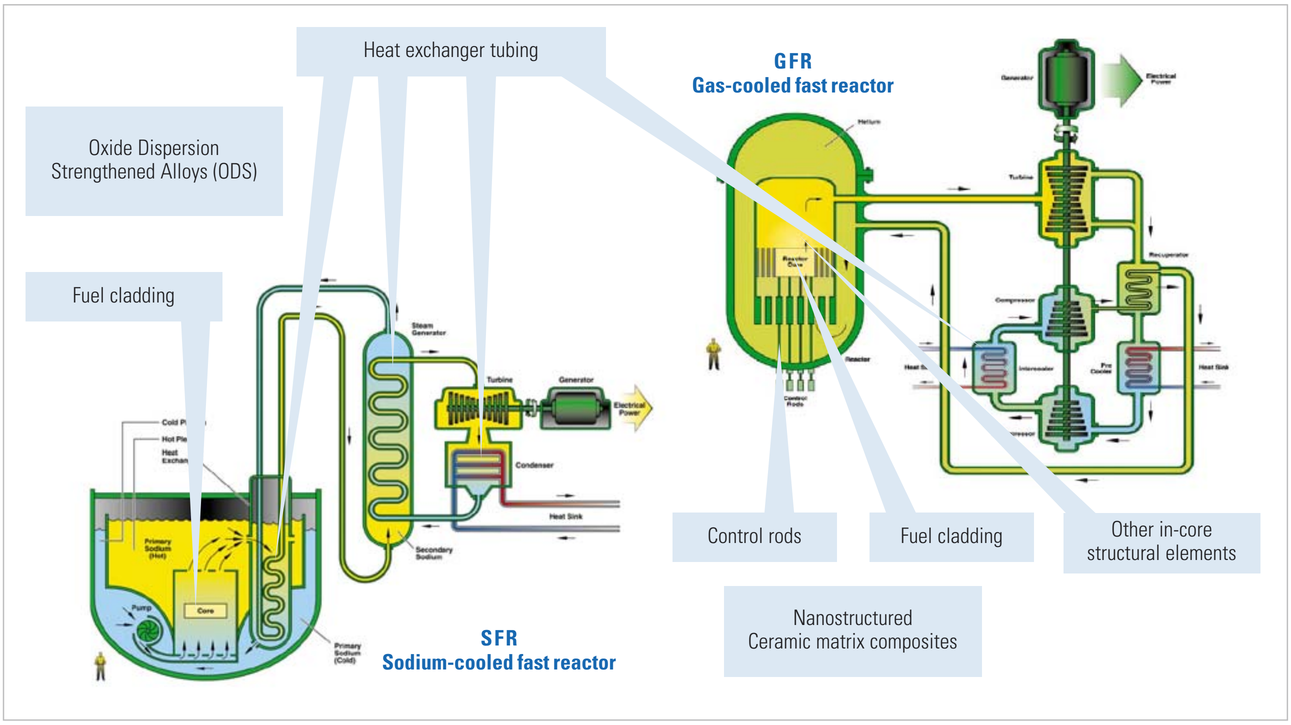


Fig. 5.5.1: Compounds where improvement is expected from the introduction of nanomaterials.

iii) The absence of heavy intermetallic phase precipitation that could degrade the toughness of the cladding.

Preliminary results under mixed and fast neutron spectra show that materials demixing should allow this type of material to keep reasonable ductility and fracture toughness. The under irradiation stability of the Oxide Dispersion is an open issue to be settled. The action of the Oxide Dispersion on the in-reactor creep, where climb phenomena are predominant, remains to be understood. Improvements will have to be reached around the distribution and stability of the reinforcements, especially with other types of strengthening precipitates.

Ceramic materials are being considered for in-core application in the GFR primarily due to the stability of their properties at high temperature. Components for which ceramics are the likely option include the reflector, control rod guides, and the upper and lower support plates. Estimates of the temperatures for the various components range from 300°C to as high as 1000°C in operating conditions, and up to 1600–1800 °C in incidental conditions. These temperatures depend on the materials used, the effectiveness of the decay heat removal system, and the core design. For all cases, the expected neutron dose is quite high, exceeding 100 dpa. Since the radiation resistance of ceramic and ceramic composite materials is strongly affected by temperature, such materials are likely to be adapted to limited regions of the core.

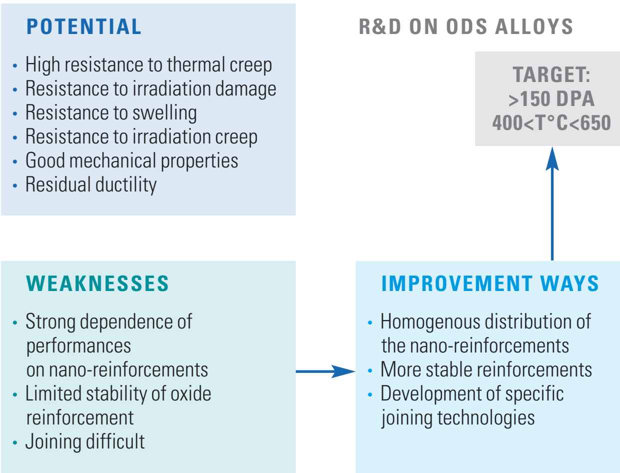


Fig. 5.5.2: Context of the research and development concerning the development of ODS alloys and similar materials.

Nanostructured ceramics are expected to present properties which will match the principal materials requirements for compounds in GFR cores. For example, they offer the possibility to undergo superplastic deformations, in contrast with their coarse-grained counterparts. Their properties related to specific surface are enhanced. Regarding resistance to irradiation damage, it is expected that their grain size will result in small diffusion distances of point defects and therefore in easier annihilation of these defects in the amorphous regions of grain

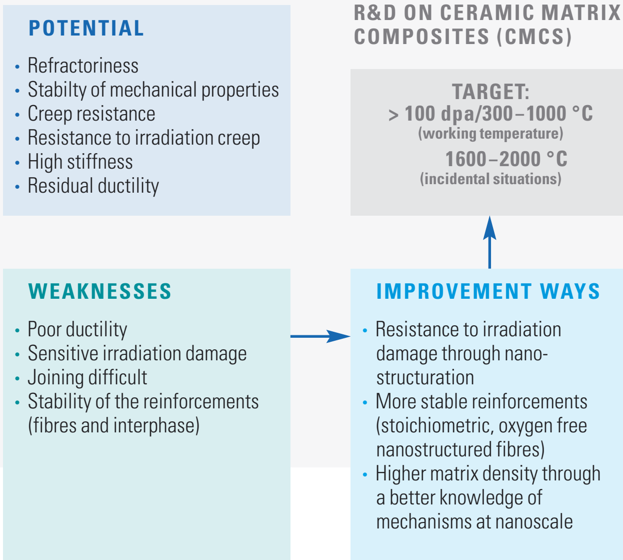


Fig. 5.5.3: Context of the research and development concerning the development of Ceramic Matrix Composites (CMCs).

boundaries, which are known to act as defect sink. The materials envisaged for GFR applications are mostly carbides, including SiC, but also TiC and ZrC for their superior thermal conductivity evolution with increasing temperature. Ternary carbides such as Ti_3SiC_2 present interesting properties that should possibly be tailored within a wide range by changing the processing parameters. Among these materials, SiC is certainly the most mature for nuclear applications since its processing as well as its properties under irradiation have already been intensively investigated, partly in the framework of the developments of materials for nuclear fusion applications. Moreover, the industrial production of SiC nanopowders has been initiated and a new start-up producing finely tailored SiC nanopowders was recently launched by the French Atomic Commission (CEA). TiC and ZrC still need more development before moving into a specific qualification program for GFR applications, not only because knowledge is still lacking about the tailoring of their properties, but also because the processing of nanostructured materials of TiC and ZrC, particularly in the case of ZrC, must be first undertaken. The case of nanostructured Ti_3SiC_2 and related ternary carbides is comparable to that of ZrC but presents additional difficulties which are related to the lack of knowledge concerning its thermal stability, its corrosion resistance in a GFR environment, and also to its behaviour under irradiation.

In the material development for GFR applications, and particularly for in-core application, the combination of a high thermal stability and acceptable fracture toughness is among the most important criteria. Most engineering alloys such as steel have an extraordinary ability to resist unstable crack propagation under load, with fracture toughness values in excess of 200 MPa•m$^{1/2}$. Following neutron irradiation, the fracture toughness for steels, as with most engineering alloys can significantly drop, though this is not of great concern unless the fracture toughness drop to values below about 30–50 MPa•$m^{1/2}$. Comparing these numbers with the fracture toughness of monolithic insulating ceramics, which have fracture toughness value on the order of 3 MPa•$m^{1/2}$., it is clear that special considerations in design are required. However, it is possible through incorporation of platelets, transformable phases (~7 MPa•$m^{1/2}$.), chopped fibres (~10 MPa•$m^{1/2}$), or continuous fibres (~25–30 MPa•$m^{1/2}$.) to increase the fracture toughness of ceramics.

Therefore, continuous fibre-reinforced ceramic matrix composites are being considered. Currently, SiCf/SiC and Cf/C seem to be the only composites of sufficient maturity to be considered for application in the GFR timeframe. However, composites with a titanium carbide (TiC) or zirconium carbide (ZrC) as matrix materials are expected to confer a better stability of thermal conductivity at high temperature to such structural composites. Concerning Ti_3SiC_2-matrix composites, their interest will strongly depend on the intrinsic properties of Ti_3SiC_2 under irradiation.

Besides the problem of developing a structural composite adapted to the GFR environment, the process will be of determining importance, since current processes used for the fabrication of such composites usually require vapour deposition techniques which are systematically related to long processing times and high costs. The development of such materials must take into account economical criteria and favour the use of simple, cheaper techniques like electrophoretic infiltration of woven fibre performs.

The development of this new generation of materials also implies a simultaneous development of the corresponding processing routes. For example, mixed oxides instead of single oxides or other types of strengthening particles have to be handled for the new ODS steels, and the nano-reinforcements are no longer only synthesised in-situ but could also be incorporated, which results in totally different routes including steps like the synthesis of these nano-reinforcements (with controlled composition, size, etc.) and their homogeneous dispersion in the matrix. Concerning nanostructured CMCs, not only the classical but expensive vapour infiltration processes will be considered, but also other techniques based on the infiltration of nanosized powders. Finally, the use of nanosized particles itself represents a challenging issue, since it results in environmental and health matters that have to be considered from the very beginning because of their impact on the processing routes.

Role of synchrotron radiation and neutrons

The development of new nanostructured materials for nuclear applications requires the development of processing routes able to ensure an improved control of the structure from the nanometric and atomic scale to the macroscopic one (up to the cladding tube for instance). For example, it is highly desirable to get homogeneous nanostructures (metallic matrix composites or ceramic matrix composites), nanoparticles, of which it is possible to adjust respectively the grain size as well as grain boundaries structure, composition and distribution in order to be able to adapt the properties of the nanostructured material "at will". The grain boundary phase can also strongly influ-

STATE-OF-THE-ART

ODS
- Oxide Dispersed Strengthened alloys (single oxide)

Nanostructured composite ceramic
- SiC/SiC materials by CVD, NITE processes
- C/C and C/SiC materials

FUTURE PROSPECTS

New generation of ODS
- Dispersion of mixed oxides in steels
- Investigation in parallel of several processing routes: in-situ reinforcement, use of nanoparticles

New kind of reinforcements in steels
- Dispersion of carbide or nitride nanoparticles in steels
- Investigation in parallel of several processing routes

Improved homogeneity
- Control of the size of the nanoreinforcements
- Homogeneous dispersion

Controlled synthesis of nanoparticles
- Synthesis of single carbide/nitride nanoparticles with well – controlled characteristics (size, structure, chemical composition)

Nanostructured composite ceramic
- Novel dense nanostructured composite ceramics (nanocomposites matrixes: Ti_3SiC_2, SiC/TiC, ZrC,... + fibers)
- Control of the grain boundary structure, composition
- Control of the grain size of the matrix in the nanometric and sub-micron range

FUTURE ROLE OF SYNCHROTRON RADIATION AND NEUTRONS

New multifunctional nanostructured materials
- Advanced characterisation (synchrotron and neutron) of:
  - Chemical and structural composition, crystallographic structures of nanoparticles (nanocomposites nanoparticles) (XRD, ND)
  - Density and size distribution of nanoparticles (SANS, SAXS)
  - Chemical and structural composition of monolithic and composite nanostructured materials
  - Interfaces and grain boundaries using imaging and tomographic analyses (XR)
  - Local stress state, microdeformation, and local texture (µ-XRD)
  - Atomic environment of "particles", Y,C... (EXAFS)
- "In-situ" experiments

Particular challenges
- High spatial resolution
- Selective chemical and structural characterisation (phases, inter-phases, grain, grain boundary)
- Correlation of the characterisations with the macroscopic properties of multifunctional nanostructured materials
- Analyses on irradiated samples

Fig. 5.5.4: Opportunities for synchrotron radiation and neutron techniques in the field of nuclear materials.

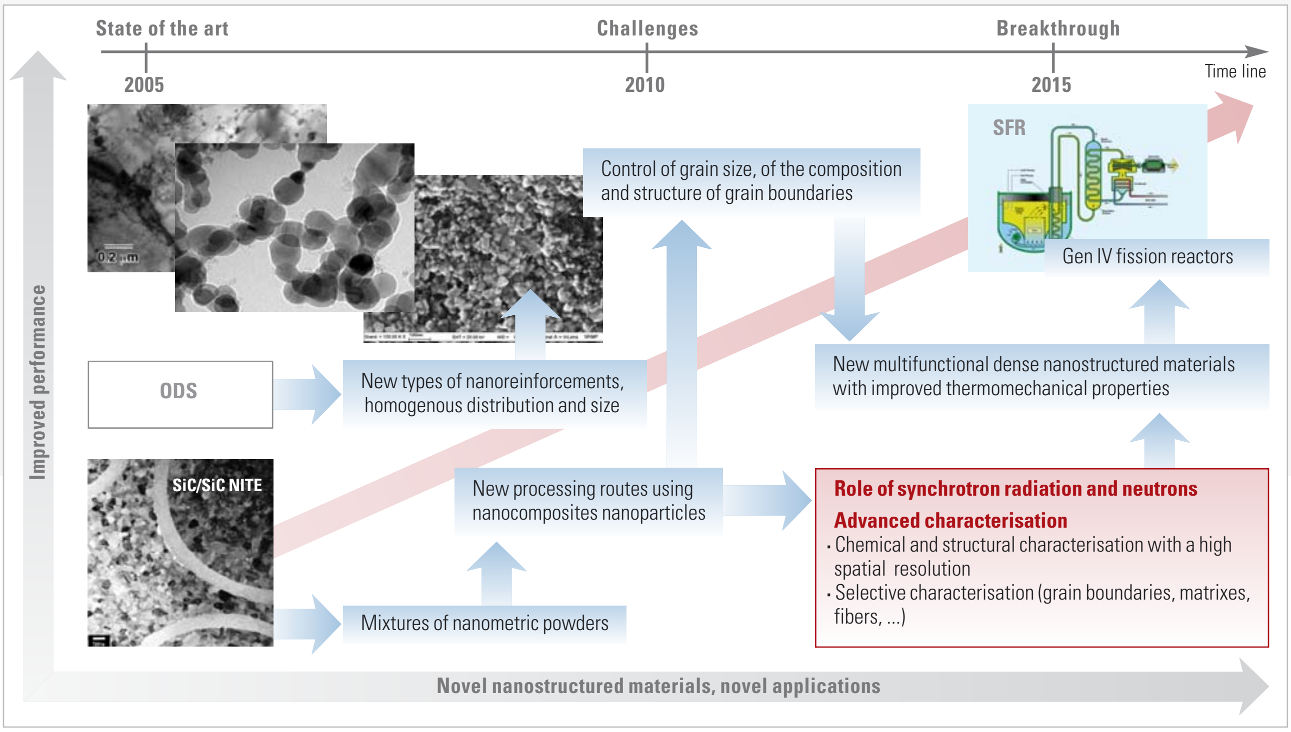


Fig. 5.5.5: Roadmap on the contribution of synchrotron radiation and neutrons and towards nanostructured materials for nuclear fission technologies.

ence thermal and mechanical properties of the materials as well as the grain size which strongly influences the properties in the nanometric and sub-micrometric range.

Consequently, it is highly desirable to be able to fully characterise the nanostructured materials developed for nuclear applications using synchrotron radiation and neutron facilities to achieve a full characterisation from the nanometric and atomic scale of the structure in the materials up to the macrocopic one. Especially since the developments of new materials tend towards a higher degree of control of the structure of the matter at the nanometric and atomic scale but also because macroscopic properties are strongly infuenced by the "nanostructuration". These techniques are complementary to usual techniques used to characterise nanostructures.

- Possibility to get a selective chemical, structural, (crystallographic) characterisation of the nanostructures. Using cross-characterisations by synchrotron radiation and neutrons, it is possible to determine radial distribution functions for a wide range of elements as a function of their environments (grain, grain boundary).
- Possibility to get a chemical and structural characterisation spatially resolved with higher resolution.
- Possibly to get density determination, size distribution for nanoparticles with a good statistic even after irradiation
- Possibly to get information on very local stress state and crystallographic textures
- Possibility to determine the chemical, structural and atomic environment of elements even at low concentrations
- Possibility to follow selectively in-situ the chemical, structural, stress state evolution of the materials
- Possibility to determine the chemical and structural evolution after irradiation (beam lines for irradiated materials). Chemical and structural stability. Determination of mechanisms of degradation from the atomic, meso- to macroscopic scale.

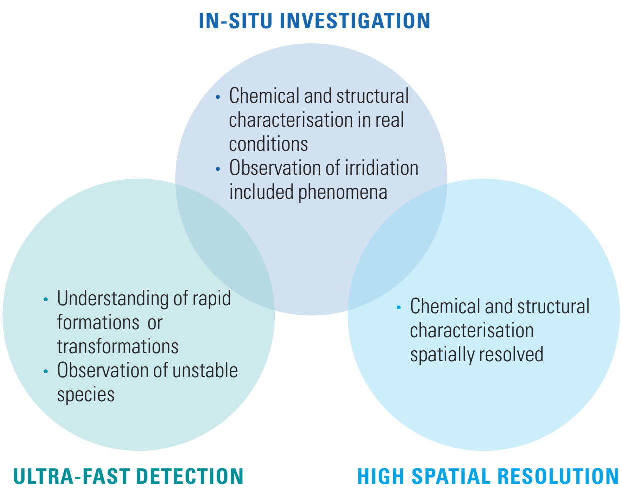


Fig. 5.5.6: Role of synchrotron radiation in the study of nanomaterials for nuclear technology.

5.5.2. NANOMATERIALS FOR FUSION TECHNOLOGY

The construction and operation of ITER will yield the most important information on fusion reactor technologies and on the plasma-material interaction processes which take place in a burning fusion plasma. Parallel to this, an intense effort is needed to develop the materials base for a fusion reactor which cannot be resolved with ITER (see Fig. 5.5.7).

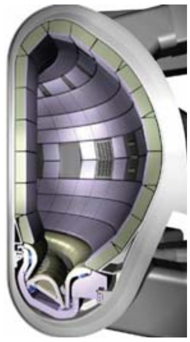
Necessary are the development of:
- Plasma-interactive materials which can sustain the power and particle loading from the plasma for an economically necessary lifetime (Fig. 5.5.7);
- Structural material for the load carrying structures which are subject to very high neutron damage doses.

These materials have to sustain extreme operation conditions, i.e. highest thermal and mechanical loads, chemical attacks and intensive radiation. To develop new materials for economically and environmentally attractive fusion energy systems, new approaches towards materials processing as well as new characterisation and testing tools are required. This poses a major challenge for the future and it requires fundamental approaches related to nanoscale processing, modelling and characterisation.

LOADING CONDITIONS FOR PLASMA-FACING COMPONENTS

BULK PLASMA
Impurity tolerance
(<10^{-5} W, 10^{-2} Be, C)

TRITIUM INVENTORY
- To be kept low (safety)
- Eroded C redeposits with high tritium fraction on 'cold' surfaces



FIRST WALL
Modest flux (10^{21} m^{2}s^{-1}) of high energy neutral particles < 100s eV

NEUTRON DAMAGE
- 14 MeV neutrons
- ITER: low dose (few dpa)
- Reactor: high dose (approx. 100 dpa)

DIVERTOR TARGET
Particle flux:10^{24} m^{2}s-^{1}
Stationary high heat flux 10 (20) MW/m^2
Transient heat loads: e.g. ELMs, disruptions: 1…10 MJ/m^2 per event

Fig. 5.5.7: Nanomaterials in a fusion reaction.

In order to reach the required degree of very high functionalisation, a nanoscopic materials engineering approach is required:
- Plasma-facing materials: The self-protection of materials against the plasma particle impact can only be obtained by nanodisperse alloying of bulk materials with passivating species.
- Barriers against tritium migration: This requires highly efficient barriers which are buried in between the plasma-facing and the heat sink material. Such barrier films have to be thin to the level of 100 nm and have a nanoscopically crystalline microstructure which is stable under intense neutron irradiation.
- Heat sink materials: In order to combine an excellent thermal conductivity with thermomechanical stability at very high temperatures, new composite materials are needed. The properties of these composites have to be tailored at the nanoscopic and mesoscopic level to optimise the behaviour of the internal materials interface.
- Structural materials: Very high operation temperatures and strength requirements lead to the need of nanoscopically tailored and stabilised materials. One path is the nanoparticle strengthening of sub-mm grain sized steels. As large quantities of the structural material will be required for a fusion reactor, the elemental composition is restricted to those elements which will not become highly activated (see Fig. 5.5.8).

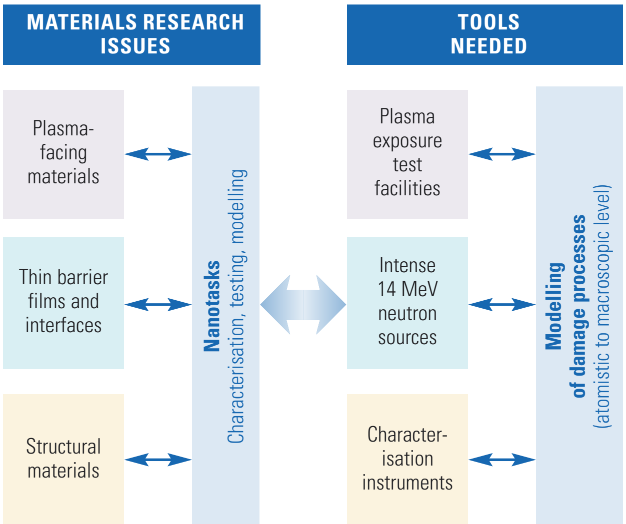


Fig. 5.5.8: Research issues and tools needed for fusion materials development.

It is mandatory to develop a detailed understanding of damage processes from the atomic to the macroscopic level resulting from plasma-surface interactions and 14MeV neutron irradiation.

An understanding of the underlying processes at atomistic and nanoscopic level will provide the key to develop new and innovative materials which can withstand the extreme operational environment in fusion. For this a basis of the following instruments and tools is urgently needed.

Future role of synchrotron radiation and neutron facilities

Characterisation tools which allow the time- and space-resolved measurement of morphology, composition, structure and strains in fusion materials on atomic to micrometre level are urgently needed. These tools shall allow the identification and quantitative characterisation of the relevant damage processes. The most important tools in this respect are: ion beam-based analysis methods, composition, structure, defect and phase sensitive analyses (e.g. XPS, XAFS, NEXAFS, PALS), microscopy (TEM, HR-SEM, AFM, STM), diffraction methods (x-ray, backscatter electrons, SR, neutrons).

In addition to synchrotron radiation and neutron technologies, a micromechanical characterisation capability is required (as push-out and nanoindentation) as well as a strong modelling activity which allows to link the observed damage with the underlying fundamental atomistic processes in a quantitative way. This will also allow to predict materials behaviour to some extent and guide the materials development. The availability of these tools will form the basis for a knowledge-based development of new materials for fusion reactor applications.

Elucidating the behaviour of hydrogen isotopes in plasma-facing materials is a key challenge:

- The microscopic understanding will lead to the identification of appropriate materials as first wall components and support the development of materials with outstanding performance in a fusion reactor.
- This requires the study of formation and hydrogen-based erosion processes in model systems by surface-sensitive diffraction techniques in well-controlled and relevant environments like UHV experiments. Neutron- and synchrotron radiation-based techniques ideally supplement the currently applied testing methods (see Fig. 5.5.9).

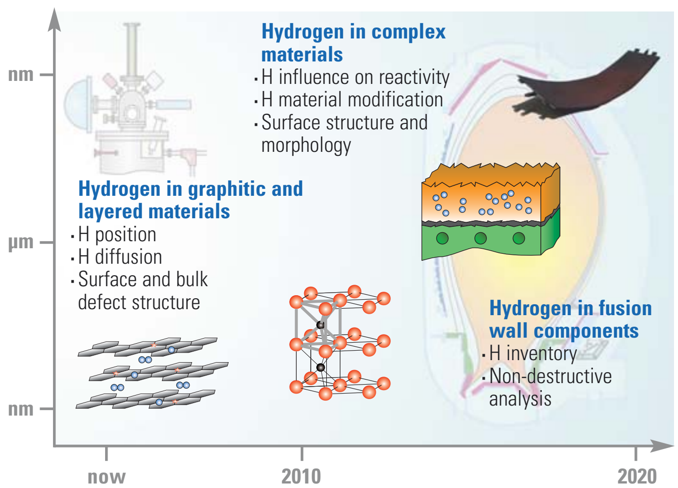


Fig. 5.5.9: Role of hydrogen in fusion materials technology – neutron and synchrotron radiation studies of model systems.

5.6. ENERGY TECHNOLOGY

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5.6.1. OVERVIEW: NANOMATERIALS FOR ENERGY

Energy resources will be vital to sustain worldwide economic growth, climate stabilisation, progress, peace, and security. New policy approaches are needed to make sure that energy supply issues do not dampen economic growth or disrupt European and global security in the 21st century. The rate of growth in energy demand worldwide runs the risk of outpacing affordable, clean supplies unless we can master not only conservation and evolutionary improvements to existing technologies but also revolutionary new breakthroughs in the energy field. So, the most important scientific- and technical challenges facing the world in the 21st century are: to protect the environment from pollution; to save resources by increasing energy efficiency; and finally, to develop efficient converters for renewable "clean" energy sources (see Fig. 5.6.1).

The different forms of energy are transported from the source to the consumer and converted to be stored and finally transformed to a usable form. Therefore, functional materials are required to convert, transport and store energy. Breakthroughs in nanomaterials and technology open up the possibility of moving beyond our current alternatives for energy supply (see Figs. 5.6.2 and 5.6.3).

Opportunities are given by nanoscale materials; in fact, all the fundamental steps of energy conversion, i.e., charged species diffusion, electron transfer, molecular rearrangements, and chemical reactivity, take place at the nanoscale. Therefore, the invention of novel nanoscale materials, and new methods to synthesise, characterise, manipulate, and assemble them, create an entirely new and exciting paradigm for developing new and revolutionary energy technologies.

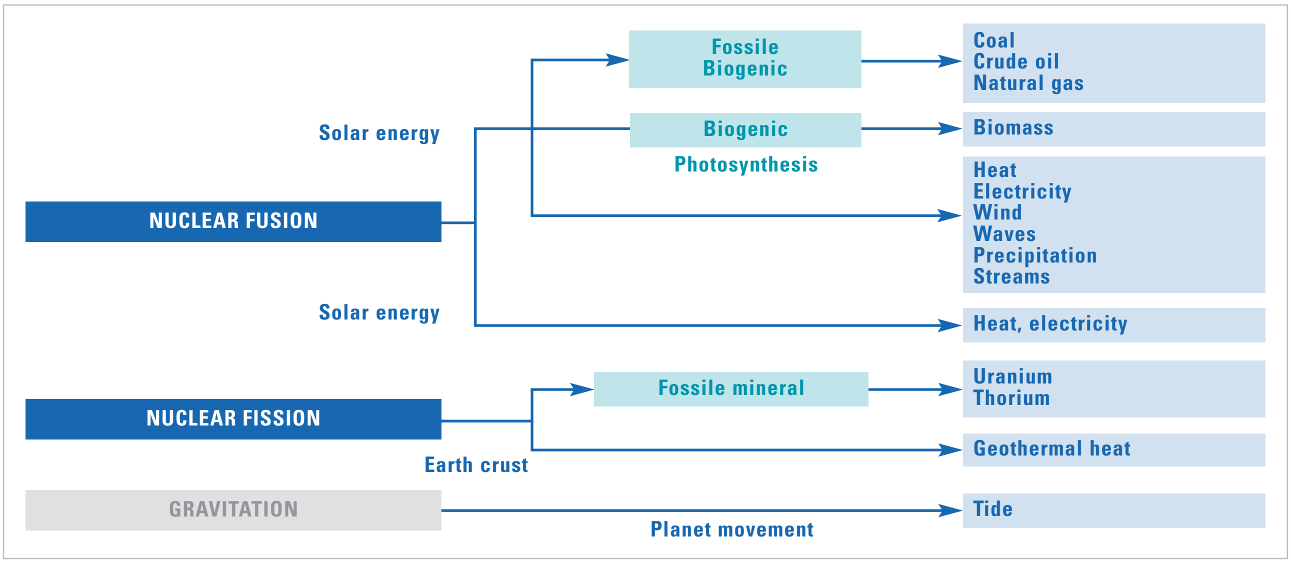

Fig. 5.6.1: Schematic representation of the energy sources and the resulting form of energy. In a fundamental sense, solar energy is the source of both fossil fuels and many current renewable energies. Solar energy in turn is the result of a fusion reaction in the sun.

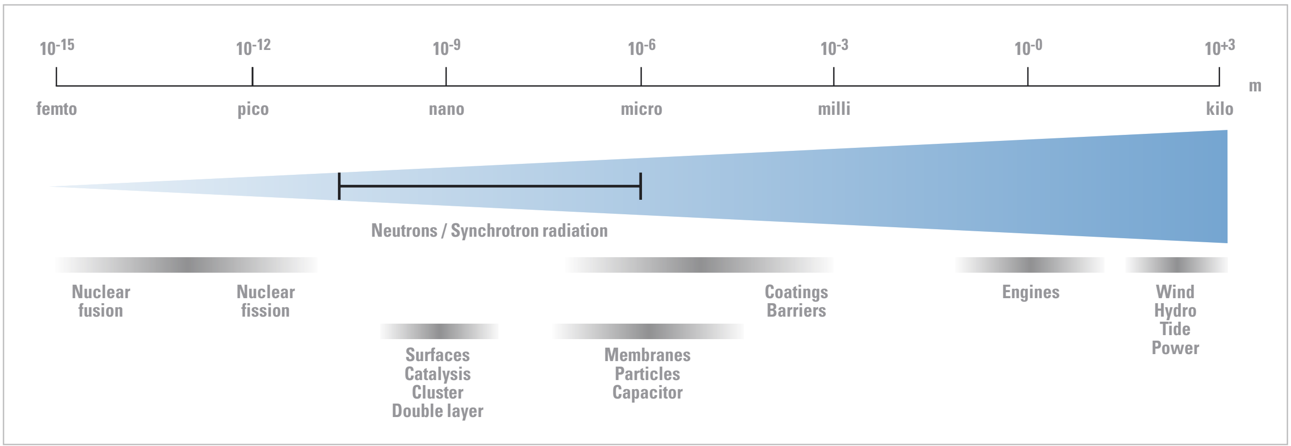

Fig. 5.6.2: Overview of the various energy relevant technologies on the length scale and the position of neutron and synchrotron radiation.

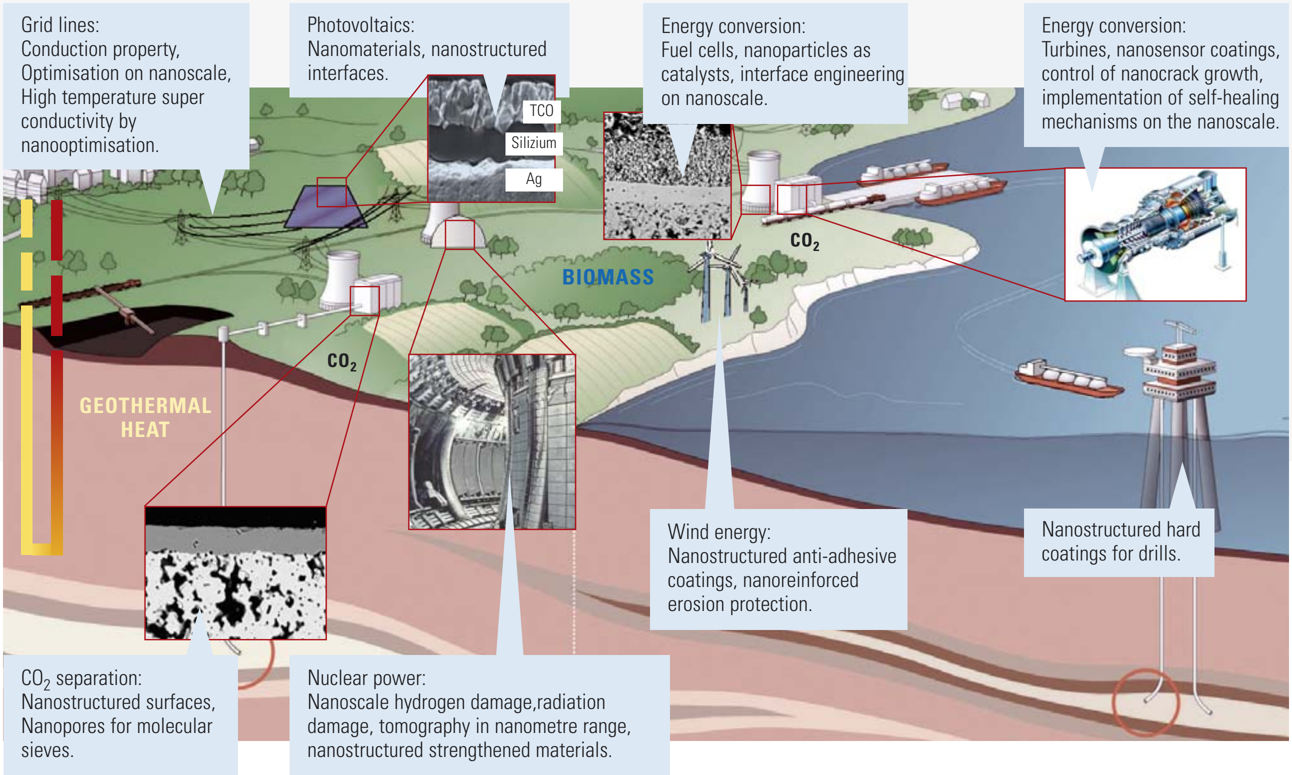

Fig. 5.6.3: Overview of modern energy technologies and the uses of nanomaterials. In addition to the examples shown, structural materials reinforced by nanoparticles are used in a large number of advanced energy converters. Courtesy: Vattenfall.

Nanostructured materials offer high potential in the area of energy technology, provided that they are well understood and tailored to exactly the right size and structure on the nanometre scale, and that powerful tools are available to characterise the produced structure. It is in this respect that an alliance between fundamental science, energy research and analysis at large research facilities will unfold its strengths.

A schematic overview of some energy chains – "sources", conversion, storage, transport – given in Fig. 5.6.4, Table 5.6.1 and Fig. 5.6.6 summarise the modern energy technologies, highlights the research needs for nanomaterials and indicates topics for which synchrotron radiation and neutron-based methods are needed for further progress. Functional nanomaterials are essential for advances in energy research: efficient energy conversion and the production of energy carriers, especially for renewable (biomass to gas or liquids) and energy storage.

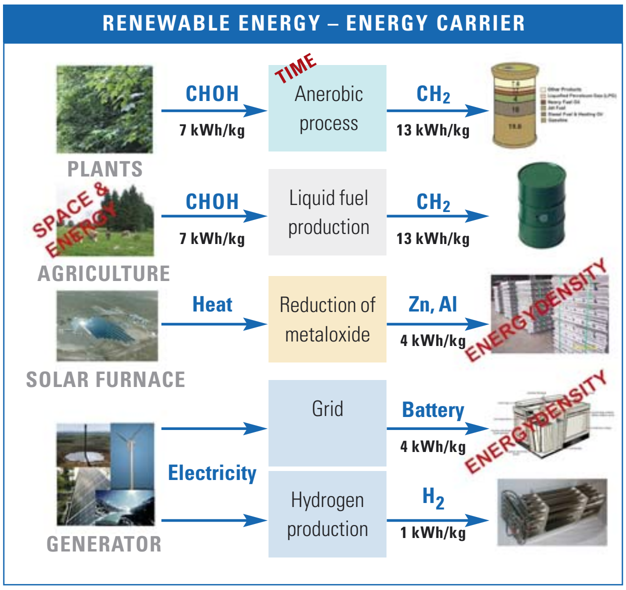

Fig. 5.6.4: Conversion and storage of solar energy in an energy carrier (from top to bottom): 1) The natural production of biomass via photosynthesis and subsequent conversion of biomass into hydrocarbons; 2) Production of biomass by agriculture and chemical conversion of carbonhydrate into hydrocarbons; 3) Reduction of metal oxide in a high temperature solar furnace; 4) Conversion of solar energy into electricity and storage in batteries or production of hydrogen.

ENERGY TOPICS		MATERIALS RESEARCH PRIORITIES	KEY BARRIERS	SYNCHROTRON RADIATION & NEUTRON RESEARCH
PRODUCTION OF ENERGY CARRIERS	Solar cells	Introduce potential of nanotechnology to reduce the costs and to improve the performance of nanomaterials.	Find new materials. Fully understand the key parameters of the performance. New morphologies (nanowires).	Characterise defects. Time-resolved experiments.
	Hydrogen	Use nanomaterials to produce hydrogen from water in using sunlight (water photodecomposition).	Find performing materials in understanding the photo decomposition true process. Integrate bio-inspired processes.	Structural and electronic structures characterisation. In operando studies.
	Nuclear fission	Consider carefully the nanoscale aspects of corrosion in nuclear power plants and the interfaces (solid-solid, solid-liquid, solid-gas) in an efficient storage of nuclear wastes.	Closely study the defects and the corrosion process. Study the solid liquid interface in lixiviation and radiolysis.	Tomography. Local structure determination. Characterisation of radioactive matter.
CONVERSION TO FINAL ENERGY	Refineries/ reformers	Develop catalysts for efficient processing of fossil fuels.	Disperse nanoparticles that are stable against sintering.	Characterise amorphous particles by EXAFS and photoelectron spectroscopy.
	Gas turbines	Increase efficiency by the use of thermal barrier coatings.	Find new materials and improve the understanding of the defects and interfaces.	Local structure determination. Tomography.
	Fuel cells	Use nanoparticles as catalysts to allow in-situ carbohydrates reforming. Develop stable membranes and electrocatalysts for fuel cells.	Understand catalytic process and interface behaviour. Understand structure and transport properties in membranes at the nanoscale.	Structure determination at various scales. In operando studies. Diffusion profiles.
	Thermo electrics	Improve the device performances in increasing density of interfaces by nanostructuring. Find new and unconventional materials. Tailor new materials at the nanoscale.	Understand the impact of the nanoscale in the performance. Obtain new materials.	Structure. In-situ and in operando studies. Defects.
	STORAGE Hydrogen	Use nanomaterials with high reacting surface with proper bonding of hydrogen.	Find new materials. Characterise the bond between H atoms and storage material.	Neutrons are very specific for hydrogen study. Structure and reactivity of the surfaces. In-situ studies.
	Batteries	Introduce nanomaterials to increase power and energy density without losing cyclebility.	Understand the role of the interfaces.	Tomography. Atomic and electronic structure. In-situ and in operando studies.
	Super capacitors	Develop new stable and performing nanostructured architectures.	Characterise surface and its interactions.	Structure. In-situ study.
CONVERSION TO USEFUL ENERGY/SAVING	Manufacturing	Develop new ways for synthesising nanomaterials of controlled size, shape and architectecture.	Study and understand the various parameters governing the species reactivity.	Follow the reactions in-situ in time-resolved experiments.
	Solid state lighting	Develop new LED's emitting light either in combining some monochromatic ones or by putting in semiconductor nanocrystals (quantum dots). Use new nanostructures (nanowires, nanotubes) and hybrid materials.	Develop and study the quantum dots to be able to incorporate them in the LED set-ups.	Spectroscopic characterisation. Structure and strain.
	Strong light-weight materials	Use remarkable properties of nanoscale phases to reduce size and weight in keeping high level of physical and mechanical properties.	Find new materials and adapt them, and existing ones, in set-ups.	Determine structural/physical properties at various length- and time-scales.
	Power transmission lines	Produce carbon nanotubes with controlled conduction properties to replace copper lines.	Manage to reach a mass production of carbon nanotubes and connect them without losing their huge electric conductivity.	Measure orientation, grafting, interfaces.

Table 5.6.1: Examples of energy technologies for production, conversion and storage and the associated key barriers.

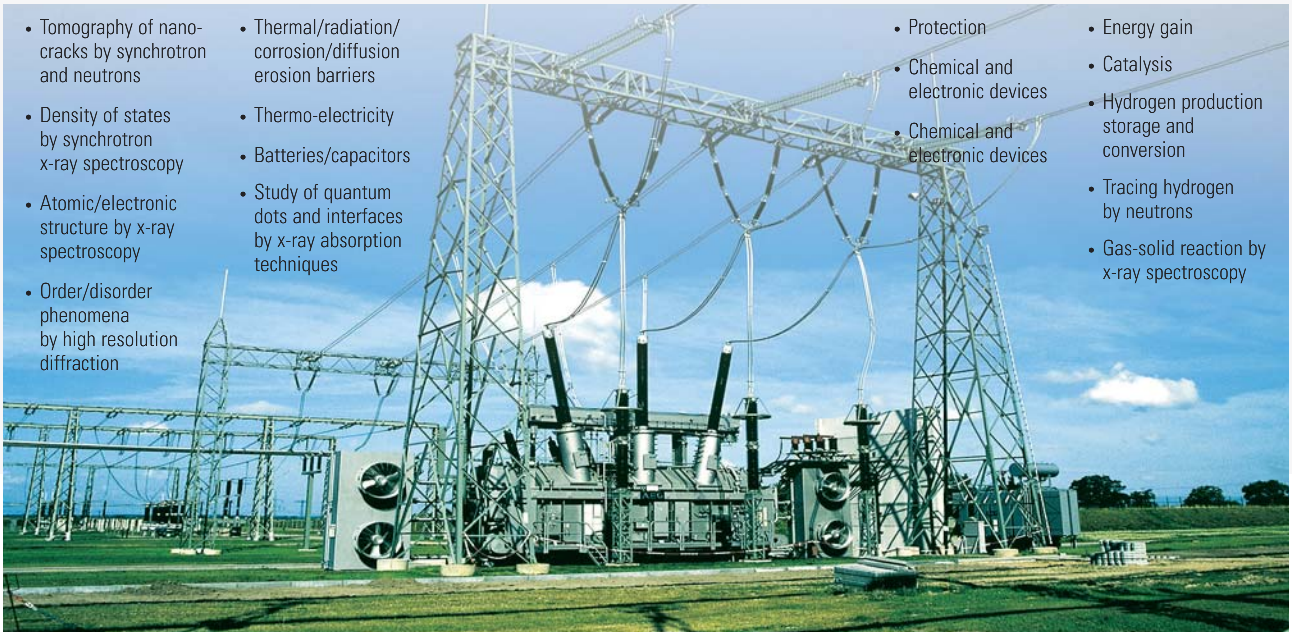

Fig. 5.6.5: Energy technologies and potential for synchrotron radiation and neutrons. For a more comprehensive survey, refer to Table 5.6.3. Courtesy: Vattenfall.

Use of large research facilities for the development of nanomaterials for energy technology (Fig 5.6.6 and Fig. 5.6.8)
The previous section was devoted to the importance of using synchrotron radiation and neutron sources for the study and the characterisation of nanomaterials for energy technologies. This section will focus on the techniques.

The availability of new, powerful techniques capable of characterising structures in the nanometre domain is indispensable for exploring the true promise of novel nanomaterials and will place energy science on the threshold of new understanding and new technology.

This will include advanced neutron-, photon-, and electron-based tools which can probe the properties of individual nanomaterials as well as the properties of nanomaterials during industrial processes, e.g., nanocatalysts under high pressure or individual nanotubes switching electrons.

A fast feedback loop from characterisation to materials synthesis is needed to understand the structure-property relationships involved, and to use this knowledge for the tailoring of nanomaterials. Information is needed about the structure on the atomic, mesoscopic, microscopic, and macroscopic (device) scales:

- Neutron and x-ray diffraction reveal the structural features at the atomic scale;
- Small angle scattering of neutrons (SANS) in polymers, and of x-rays (SAXS) for microscopic carbons and oxides, are used to reveal the ordering on the "mesoscale" ranging from a few to a few hundred nanometres, which is often decisive for the mentioned functions mentioned, such as self-ordering phenomena;
- Neutron and x-ray microtomography and radiography are used for the imaging of microscopic features;
- X-ray absorption spectroscopy (EXAFS and XANES), x-ray photoelectron spectroscopy, and inelastic neutron scattering are tools for chemical characterisation (e.g., on oxidation states and surface functional groups). This analytical knowledge is needed for converters and storage materials on top of the structural data.

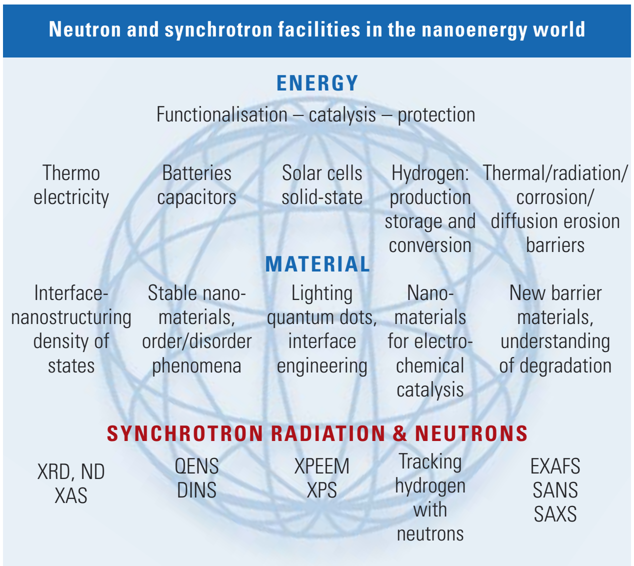

Fig. 5.6.6: Overview of the research needs in nanoscale energy technology.

Characterisation at large research facilities – indispensable for nanomaterials development in energy research

DIFFRACTION AND SCATTERING
Essential tool for structural elucidation

SMALL ANGLE SCATTERING
Shedding light onto the important mesoscale

XAS
Instrumental for materials without long-range order, such as batteries, catalysts

SPECTROSCOPY
Indispensable for chemistry, kinetics

IMAGING
direct evidence for structure "seeing is more than believing" both indirect and in reciprocal space
Large facilities will shed light on nanostructures for energy research

Fig. 5.6.7: Characterisation at large research facilities for nanomaterials development in energy research.

Specific research themes where large research facilities will provide a major impact:

- Electricity generation: develop nanodispersed and nanocomposite materials for ultrahigh temperature operation leading to dramatic efficiency increase;
- Synthetic fuels: develop stable, highly active nanosized catalysts for the production of high performance synthetic fuels by gas-to liquid, biomass-to-liquid and other chemical processes; the development of nanosized catalysts or nanosized additives on existing catalysts for producing hydrogen with sunlight.
- Storage materials: develop: i) nanostructured materials which store hydrogen or electricity at superior energy/mass, energy/volume ratios; ii) nanostructured positive- and negative electrodes for advanced batteries (such as lithium charge transfer batteries); iii) nanoporous, high surface area carbon materials for achieving the giant charge storage capacities of super capacitors, up to 100 F/g; iv) nanostructured carbon materials with exceedingly high surface area; v) complex metal alloys/hydrides where hydrogen is stored on interstitial sites.
- Fuel cells: increase performance and reliability while lowering the cost; develop and characterise nanostructured catalysts, membranes, diffusion layers, reactant distribution and cooling systems.
- Electricity transmission: development of advanced compounds.

Challenges in the further development of large synchrotron and neutron research facilities for energy technology

- Characterisation of nanomaterials in simulated energy industry environments will allow important direct investigations of the time- and temperature stability of nanocrystalline phases.
- Insights into the structural evolution of nanophase materials under stress may allow for an understanding of the origin of the often-observed increased strength with decreasing grain size.
- Studies of deuterated metals will yield insight into embrittlement phenomena in nanoscale materials.
- Real-time studies of the nucleation and growth of nanocrystalline materials from nanocrystalline precursors.
- Non-destructive studies of the precipitation of nanocrystalline phases within bulk materials at high temperatures.

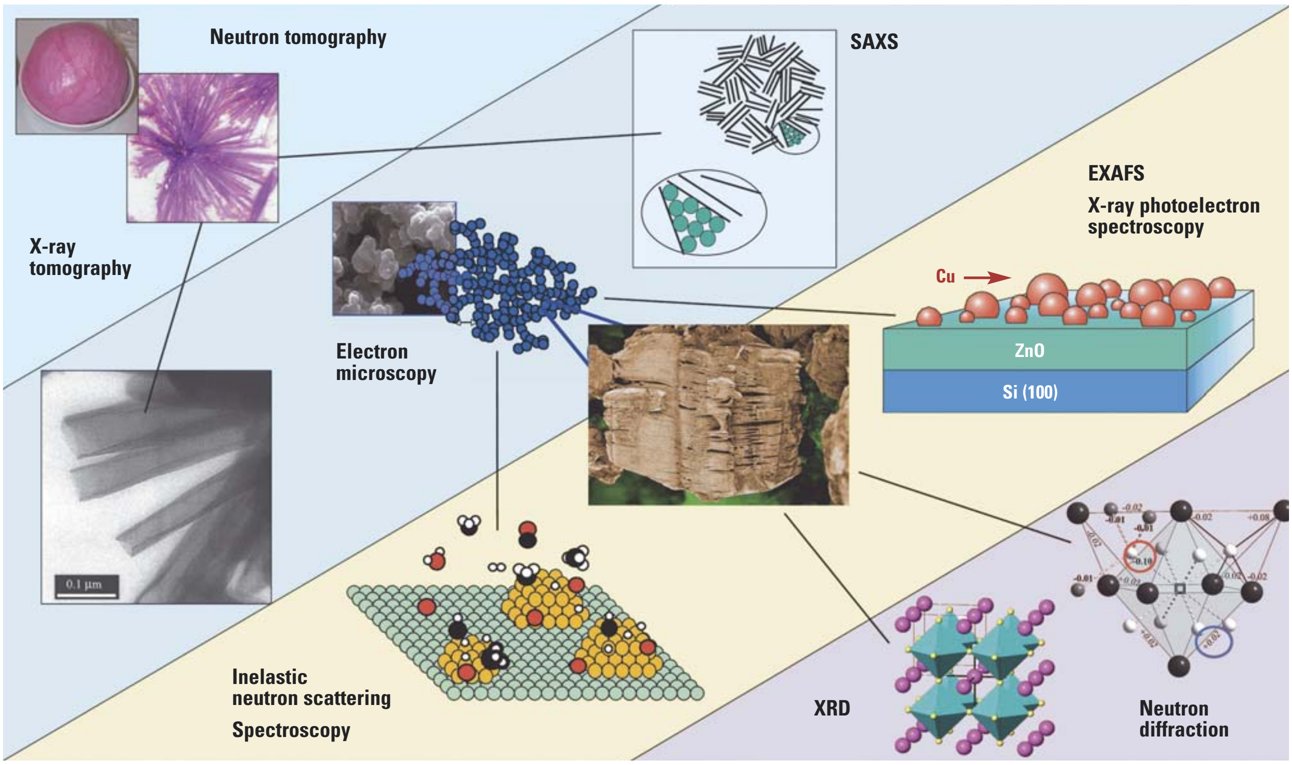

Fig. 5.6.8: Neutron and x-ray diffraction reveal the structural features at the atomic scale.

- Quantitative examination of hydrogen and/or hydrogen storage in nanocrystalline materials.
- Studies of catalysts in real-world application environments to understand both their activity and the technologically important relationships between nanoscale structure and catalyst performance.

In order to advance in the development of nanomaterials for energy technology and to attain the ambitious target specifications for energy technology, the characterisation tools must advance according to:
- Sources: "increase source intensity" – "high-brightness" – "enhance microfocusing capabilities";
- Detectors: "enhance spatial resolution from mm to µm to nm" – "increase time resolution for the study of ultra fast processes from us to ns to ps to fs".

Higher intensity and/or higher brightness of the sources is needed in order to: i) be able to detect and characterise smaller features or components present in small weight fractions; ii) enhance the microfocusing capabilities for characterising heterogeneous materials; iii) enable the studies of nanomaterials at work i.e. individual nanotubes in an electronic or photonic device.

Sample environments must be developed to study the functional materials in-situ under conditions simulating industrial operating environments; for which the design requires a close link between the beam line scientists and the users,

Enhanced time resolution of sources and detectors are required to follow structural changes during cyclic or long-term operation, for establishing materials reliability. Microsecond resolution is required for fast chemical processes, whereas elementary chemical reactions occur on the nanosecond and picosecond time scales, and excitations in solids often require femtosecond time resolution;

Increased spatial resolution of the imaging methods, in order to extend the real-space mapping of structural features from the millimetre range (standard) to the micrometre range (standard with x-rays, being approached with neutrons) and further to the 10–100 nm domain; x-rays and neutrons do ideally complement each other in imaging due to the differences in cross sections for specific elements;

Increases in spectral resolution by at least one order of magnitude to reveal changes in chemical bonding or oxidation state that are crucial for the functioning of surface active materials.

In summary, the targets for nanomaterial functional specifications are as ambitious as those formulated for source specifications, but it is only by the concomitant development of both that the desired advances of energy technologies towards a more sustainable energy system can be achieved.

European Nanoscience Energy Centre

At present, in Europe, scientific inquiry in the energy arena is scattered and diversified, with many research groups working separately towards different pursuits which lack a clear roadmap to a better energy future.

The breakthrough in the energy issue in Europe is strongly linked to the discovery of new nanomaterials for novel, efficient and environmentally-friendly energy technologies. Achieving this target requires a bundling of brilliant scientists and the availability of an excellent platform of scientific equipment. The most profitable way is to create a European Nano Science Energy Centre, where the criteria for success would be available. In view of the Large Test Facilities existing or under construction in Europe, a virtual centre or network might be the most appropriate form of organisation. This European Centre should have a nanoscience programme for energy technology working in close collaboration with regional- and/or national energy science and technology centres and universities of excellence throughout Europe. In order to improve the impact of synchrotron radiation and neutrons in the development of use and understanding of nanomaterials in the energy domain, it is important to create a Centre which will closely link energy research with the large scale facilities which are essential to its vital development (see Fig. 5.6.9).

This Centre will unite, with excellent access to synchrotron and neutron sources, prominent researchers in the nanomaterials synthesis and processing, surface and interface characterisation, physical characterisation, theory and modelling; electrochemistry, charge transport, and other disciplines mentioned in this report. Modern equipment traditionally found in materials research, such as chemical synthesis and preparation, basic analysis techniques (elemental, SEM, TEM, EDX, surface area, porosimetry), and transport measurements, will be available to the research groups participating in the Centre.

This Centre, besides developing its own research agenda, will provide the help and connection to external researchers interested in using synchrotron radiation and neutron facilities for sample preparations, human and technical support for experiments, support in data

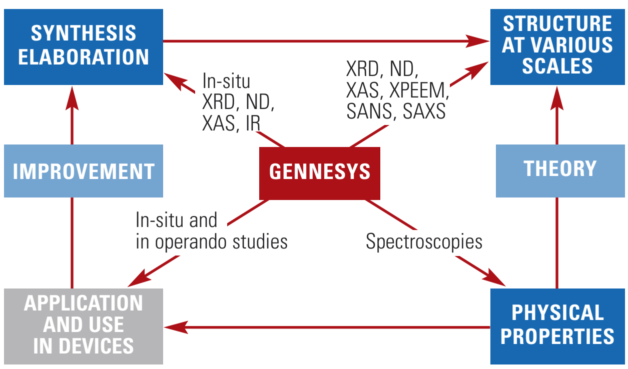

Fig. 5.6.9: Layout of a European technology centre for nanomaterials for energy technology.

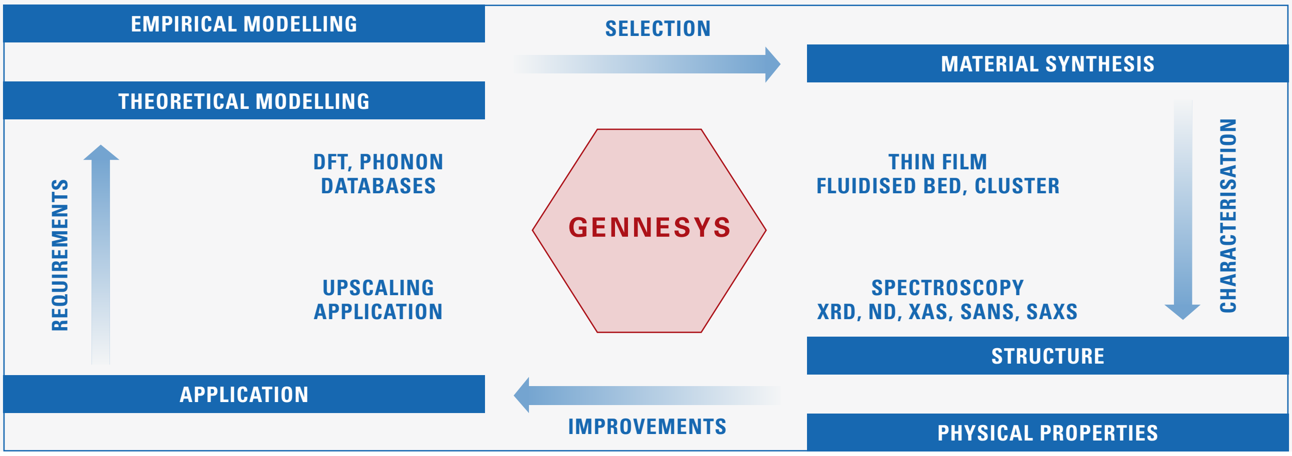

Fig. 5.6.10: Research portfolio for a European centre for nanomaterials.

treatment, training in use of facilities and data exploitation. A typical research portfolio is illustrated in Fig. 5.6.10.

Conclusions

A breakthrough in energy technology demands for nanomaterials science: syntheses, characterisation, phenomena and properties modelling. This new science era will ensure economical and at the same time safe, durable, reliable and environmentally-friendly energy conversion systems for the future. This science is still in its infancy and in order to make revolutionary progress which is of utmost importance for Europe, a European centre of excellence is to be set up. Synchrotron radiation and neutron sources based analysis techniques offer tremendous progress in investigating nanoscientific research; so it becomes clear that such European Centres should be set up at the locations of national research centres, locations where great competence in physics, chemistry, biology, and materials sciences is equally available. In addition, these national centres boast a large spectrum of advanced classical equipment.

For the major topics of fuel production, energy storage, energy conversion, and waste management, Table 5.6.2 indicates exemplary research questions for which synchrotron radiation and neutron based methods have been proven as major sources of information, and are urgently needed for further progress.

The main message of this chapter is summarised in Table 5.6.3, which represents important steps of full energy chains in the columns, and synchrotron as well as neutron based characterisation tools in the rows.

Entries in Table 5.6.3 show emerging energy materials which contain nanoscale structures, and the properties that need to be characterised at large research facilities. The main message is that synchrotron and neutron-based techniques at large research facilities will be indispensable for progress in the development of nanomaterials for new and advanced energy technologies. Highly active and selective catalysts for fuel production, high surface area materials for physical, chemical,

MOTIVATION	MEASURE	NANOTECHNOLOGY ASPECTS	IMPORTANCE OF SYNCHROTRON RADIATION AND NEUTRONS
Efficient energy conversion	Protective coatings Fuel cells	Nanoparticles, nanosensors Nanostructured polymers	SANS/SAXS/ASAXS analysis of nanoscopic changes, detection of light elements
Clean environment Renewable energy	Gas separation membranes Photovoltaics Solar thermoelectric conversion	Nanometre-tailored ceramic proton, ceramic oxygen, ceramic mixed micronanoporous ceramics Thin poly-, micro- and nanosystems/ interfaces	SAXS/SANS/EXAFS analysis of oligomers, chemical analysis, XPEEM for detection of local chemical and structural information, XPS, XAS
Fusion	First wall materials	Chemical and structural analysis, protection concepts	Detection of light elements in heavy element matrices by neutron spectroscopy
Energy storage	Accumulators, capacitors	Nanostructure-property correlation in active electrode materials	Following atomic-scale morphological changes/ nanoscale disorder by SANS, QENS and DNS

Table 5.6.2: Research portfolio for a European centre for nanomaterials.

or electrochemical energy storage, structural materials for highly efficient energy converters, and advanced waste management schemes all depend on structures and properties that are tailored at the nanometre scale.

It is here where the power of analytical tools available at the large research facilities can make a decisive difference. Diffraction and small angle scattering methods, using both x-rays and neutrons, provide structural information at the atomic and at the nano-/mesoscopic scale. Insight into chemical states and bonding becomes accessible from x-ray and Vacuum Ultraviolet Spectroscopy. The increased spatial resolution of next generation sources will advance imaging to a previously unaccessible level of detail. Higher intensity sources with superior time resolution will be used for operando studies of the relevant components, and for investigation of the important time-dependent materials. The novel functional materials emerging from this productive feedback loop between innovative synthesis/ development and powerful characterisation will be the key in the progress towards a more sustainable energy system comprising fuel production, energy storage, and efficient conversion.

A schematic representation of the energy sources with conversion technologies, energy storage and transport, and energy saving is given in Fig. 5.6.11. The second part of this chapter describes the future research needs for the different energy technologies and highlights the importance of the use of synchrotron radiation and neutrons in order to achieve breakthroughs.

	FUEL PRODUCTION	ENERGY STORAGE	ENERGY CONVERSION	WASTE MANAGEMENT
DIFFRACTION	State and dynamics of catalyst structure	Structure, phases of storage materials	High temperature materials, nanocomposites	Corrosion; advanced waste treatment
SANS/SAXS	Enhanced oil recovery; hydrates	Nanoporous materials, active carbons	Fuel cell and gas separation membranes	Clay materials
XAS	Catalyst nanoparticles, surface alloys	Redox processes in batteries, electrolytes	Thermoelectrica; in-situ characterisation of catalysts	Metal binding to sorbents, multi-barriers
SPECTROSCOPY	Catalytic reaction mechanisms	Electrode surface processes, superconductors	VUV spectroscopy of combustion processes	Identification of elements, speciation
IMAGING	Microreactors in operando	Phases and grains in complex alloys	Working fuel cell stacks, engines	Visualisation of slow diffusion processes

Table 5.6.3: Nanomaterials for energy applications – characterisation at large research facilities.

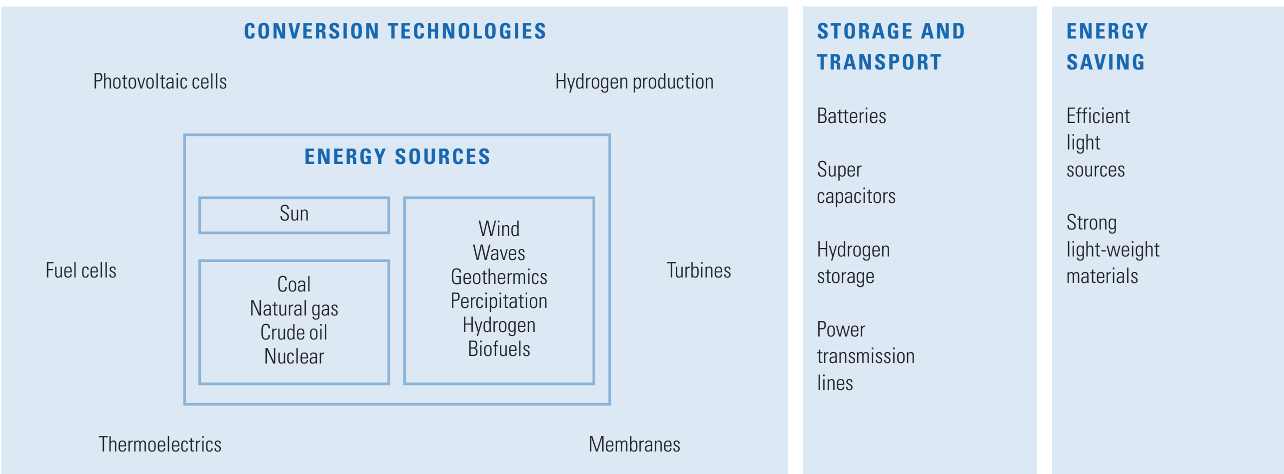

Fig. 5.6.11: Schematic representation of energy sources with conversion technologies, energy storage and transport and energy saving.

5.6.2. ENERGY PRODUCTION

Biofuels

As the energy used in transportation has to be storable, of high energetical density, and compatible with gasoline or diesel engines, 93% of it comes from oil and a little more than half of the global oil production is used for that purpose. At the global level, in 2005, emission of CO_2 in transportation applications was 24% of the total CO_2 emissions and it is sharply increasing. Biofuels, if produced in sustainable conditions, can help to mitigate greenhouse gas emissions and in the future provide about 10–20% of the total fuel needed for transportation.

Biomass has always been used by men for food, bio-products and transportation. Biofuels are an example of an application used today (Fig. 5.6.12).

(a) First generation biofuels

First generation biofuels are those used today. They belong to two families. The first one is based on crops containing a high concentration of sugar such as sugar cane, sugar beet, sweet sorghum or starch such as corn, wheat, barley. Yeast fermentation produces ethanol which can be used directly or in turn can be transformed into other products like ETBE, and then can be blended with gasoline. The second family is based on plants such as oil palms, soybeans, rapeseeds, sunflowers which contain a high concentration of vegetable oil which can be used as biodiesel, either directly or after methylesterification to be blended with standard diesel oil.

The main concern with first generation biofuels is that a wide use of them could compete with food biomass. In addition, most of the crops used to produce them need fertilizers, or a large quantity of water. Their CO_2 balance is also quite poor; nevertheless, it is always positive.

(b) Second generation biofuels

Second generation biofuels use lignocellulosic biomass (wood, forestry and farming residues, waste biomass, dedicated non-food crops). Dedicated non-food crops can be perennial grasses such as Miscanthus, short rotation coppices or undergrowths. There are two ways to process lignocellulosic biomass. The first one is to make cellulosic ethanol using biochemical reactions. The second one is to

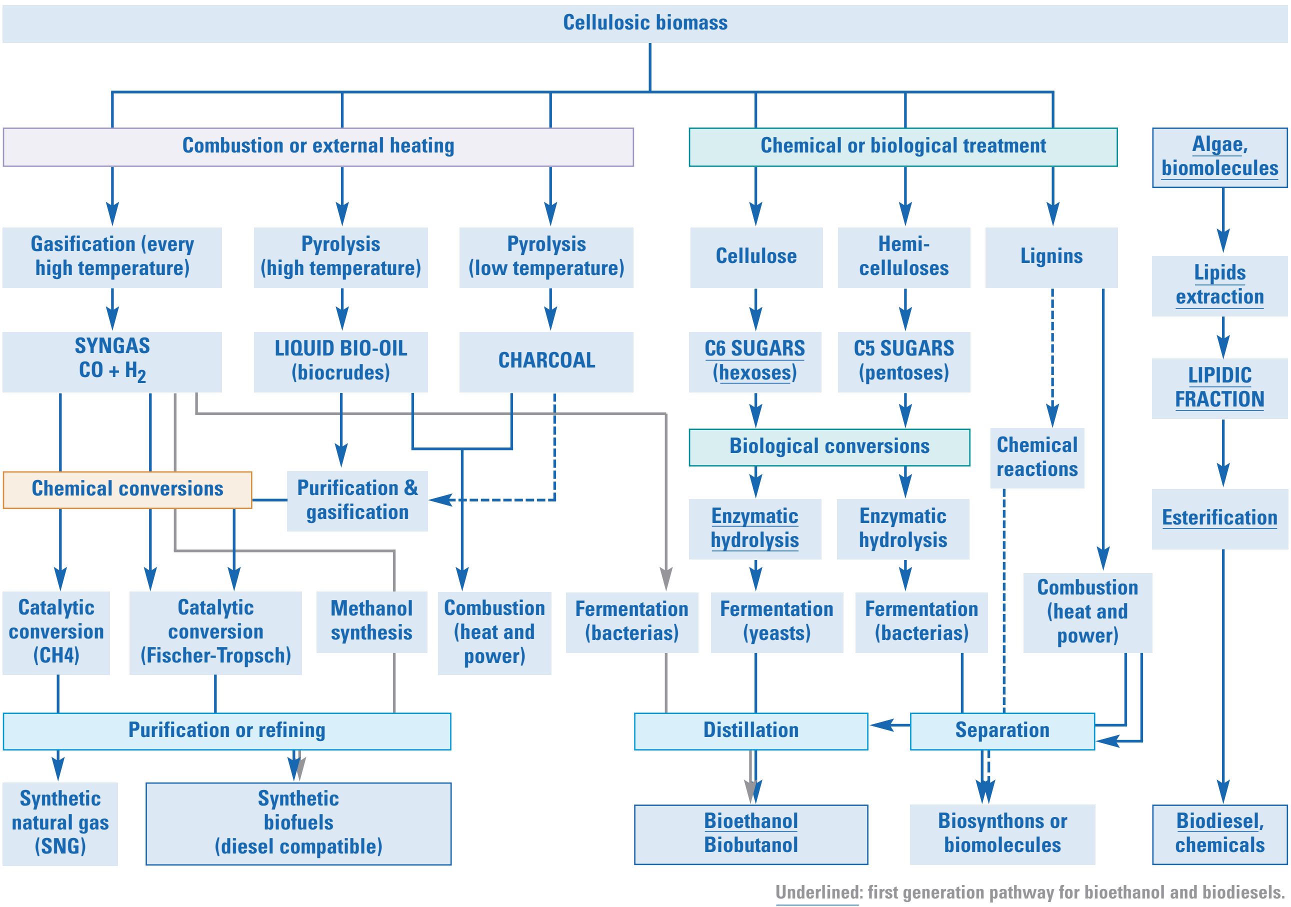

Fig. 5.6.12: Overview of biomass transformations leading to first, second and third generation biofuels.

transform biomass after gasification into liquid fuel using the Fischer-Tropsch process.

Woody and fibrous biomass contains cellulose, hemicellulose and lignin. The main challenge for implementing the biochemical pathway is to be able to develop efficient ways for adequate separation of these three components, and micro-organisms transforming hemicellulose into ethanol with a good yield. Genetic engineering or selection should allow to produce biomass with less lignin and/or with cellulose, hemicellulose and lignin structures which are easier to be transformed by biochemical reactions.

The thermochemical way is close to industrial application. This route is known as BTL (biomass to liquid) and produces very pure diesel oil. Its main challenge is to minimise energy losses and maximise fuel yield. If external energy and hydrogen produced without CO_2 emissions are used to garner all the carbon available, in the end, one can get 2 or 3 times more synthetic oil per surface unit with BTL than with crops used for the first generation biofuels.

(c) Third generation biofuels

In the future, biofuels could also be produced with aquatic micro-organisms. Oil from micro-algae is currently explored as one of the most promising ways to produce biodiesel. One advantage is that the yield is one order of magnitude larger than for oil seeds cultivated inland. Another important advantage is that there is no competition with food crops. Furthermore, algae can be continuously harvested and could be used coupled to an industrial facility emitting CO_2: instead of directly emitting CO_2, oil can be produced, thus improving the energy to carbon ratio of the overall process.

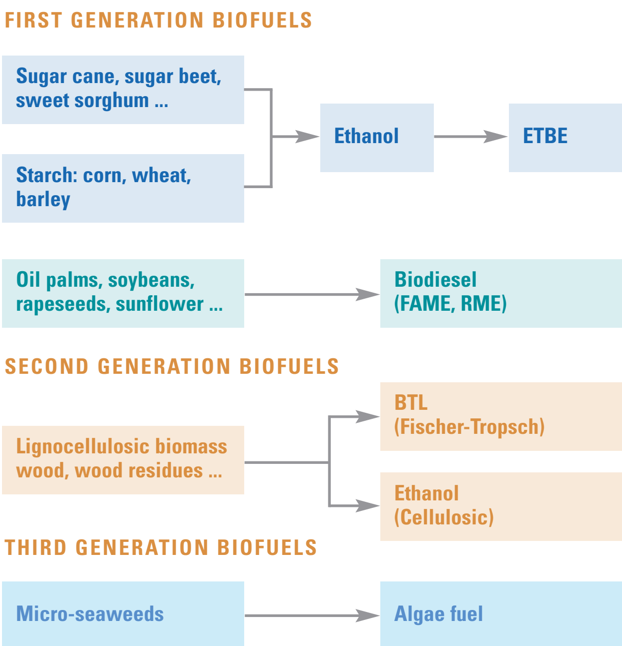

Fig. 5.6.13: Biofuels generations.

There are between 200 000 and a million different species of algae. Some of them can grow in extreme conditions. Several micro-algae have been found to produce oil with a much higher yield than oil seeds cultivated inland (Fig. 5.6.14). Note however that with current practice, conditions that lead to high biomass yield are different from those which lead to high oil content, and that maximum yields have been obtained in controlled conditions which are difficult to scale up. It is a major challenge for current research to identify strains and conditions which will combine high biomass, high oil content, and robust/inexpensive cultivation.

Developing algae oil at an industrial scale is an important issue for Europe since transportation is mostly based on petroleum products; in Europe at least France, Germany, Great-Britain, Malta, Netherlands, Portugal, Italy and Spain are working on this long-term subject. In the USA, the DOE has estimated that, potentially, an area in the sea of the size of the state of Maryland could provide enough biofuel to replace oil used in the USA.

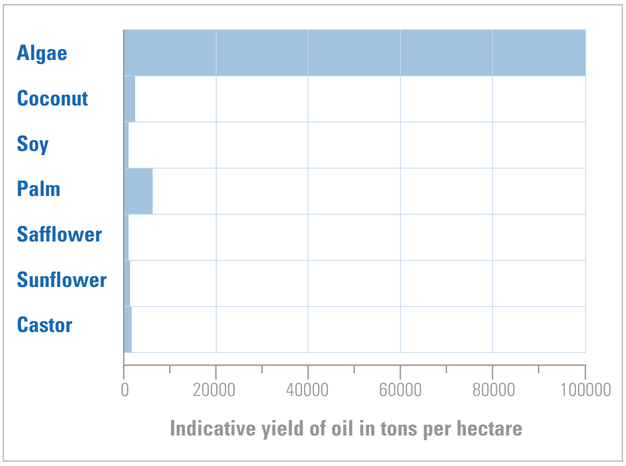

Fig. 5.6.14: Indicative maximal oil yields for various oil seeds and algae.

Which strategy for biofuels?

It is urgent to develop second generation biofuels at an industrial scale and to push research on third generation biofuels (algae fuels).

As far as entire earth or marine plants are concerned, all parts of the plant should be used in one way or another and not only a part of it as it is done today in most cases. Genetic modification technologies together with nanotechnologies and modelling are needed to improve plants and tailor dedicated earth and marine crops. Gathering valorisation modes for a given biomass type i.e. combining: (i) extraction of high value compounds, (ii) use of edible or other directly valuable products and (iii) biofuel generation, will certainly be one of the best ways to initiate economically relevant bioenergy producing units (so-called "biorefineries").

Micron-size plants (algae, cyanobacteria) with specific production potentials should be identified, both in marine and freshwater areas, and genetically improved. These plants could be grown out of soil in marine areas, in ponds or on non-arable land in specific photo-reactors.

In general, tailoring dedicated crops and developing more powerful micro-organisms and thermodynamical processes are key issues to make biofuels economically competitive and environmentally-friendly.

- **Research needs in nanoscience and nanotechnology**
  Nanosciences, genetically modified crops and nanoscale characterisation can help improve the production of biofuels while decreasing the cost at three different steps in the whole process:
  - Production of selected biomass;
  - Improvement of industrial processes;
  - Nanoscale or microscale characterisation of chemical reactions.

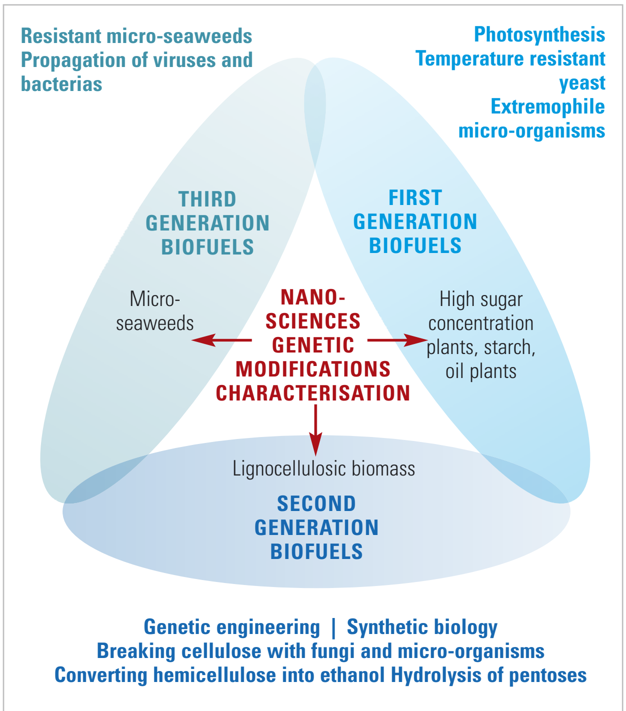

Fig. 5.6.15: Global view of research priorities in nanosciences for biofuels.

There are also other domains in which nanotechnologies can play a role together with macroscopic approaches. We shall briefly go through the needs.

(a) Production of biomass

As the production of structured biomass is achieved by agriculture and forestry and has to be done with a high level of sustainability, all the research needs for these sectors (see 5.3.6 Agriculture) are also relevant for biofuels. Among them, these are the most important:

- Knowledge and control of the structure of plants by identification of genes and enzymes responsible for the synthesis and assembly of plant cell walls, in order to facilitate their transformation and optimise their composition: easiness to fractionate, high level of positive components, reduction of ashes etc.;
- Increase productivity while keeping sustainability with three major long-term key issues: efficiency of photosynthesis, optimised use of nitrogen (slow release fertilisers, nanosystems for using nitrogen from air, etc.), reduction of biomass losses (nanoparticle pesticides, nanosystems for preservation during storage, etc.), reduction of water loss.

(b) Characterisation and improvement of biological processes

The biological transformation of biomass is something that is undertaken by life processes themselves. For the biological production of biofuels, the key issues are to accelerate these processes and to route them towards molecules usable for energy production, like alcohols, lipids or hydrogen. Such objectives could be obtained through:

- Comprehension of interactions, at the nanoscale, of biocatalysts with their substrates and their inhibitors, and with the products of the reaction : improved knowledge of lignocellulose-imposed limitations for enzymatic catalysis like diffusion and/or interactions with cell wall components;
- Specific design, by protein engineering, of biocatalysts to add some new functionalities to them or to favour some properties (catalytic efficiency, resistance to heat and pH, for instance);
- Intensification of processes via nanoscale reactors or contactors, in order to increase the speed of diffusion or convection processes;
- New systems for being able to recycle biocatalysts and/or micro-organisms, while their present use is generally disposable;
- New methods for high-throughput screening of lignocellulose digestibility, to be used, for instance, in metagenomics approaches;
- New sensors using nanotechnologies for improved control of biological reactions, when they are implemented on industrial scale installations.

(c) Characterisation and improvement of thermochemical process

The thermochemical process is performed at elevated temperature, far above life processes temperatures and kinetics. The key issues are the strict coupling between mechanical, thermal, hydraulic and chemical areas in fast thermochemical reactions. Main pollutants have to be reduced to avoid catalyst poisoning. Biomass and organic waste variability have to be smoothed. Such objectives could be obtained through:

- Comprehension of thermally weak molecular links in the biomass;
- Prediction of organic products release, yields and composition;
- Prediction of inorganic compounds state and links in the biomass, release, yields and composition;
- Production of resistant nanoscale catalysts and adsorbants, separation and recycling;
- Comprehension of catalyst and adsorbants chemical action;
- Elaboration of nanoscale sensors to improve the control and measuring of reactions and low level of pollutants.

(d) A better use of micro-algae

There are still many problems to solve before reaching an industrial stage of producing biodiesel from algae and research is urgently needed. Studies about the impact of cultivating micro-algae in great quantities are required. It is also necessary to find the optimal conditions for growing and selecting the right species. For example, the yield dramatically decreases with too low or too high temperature. Stability and resistance against microbes of viruses are important issues if large areas are cultivated. Infection by other algae species might also be a problem. Genetic engineering will play a key role in this research. It is at this stage that nanotechnologies and characterisation using neutron scattering and synchrotron radiation come in.

- **Biological research roadmap**

2008–2012

- To study the structure of plants at the nanoscale and the influence of genetic and external variables like cropping conditions;
- To study the diffusion and interaction at the nanoscale of enzymes in plant cell walls and biomimetic systems;
- To develop new tools for understanding the plant cell wall structure at the nanoscale, and cell wall accessibility and limitation to biocalytic processes;
- To study the possibility of adding new functionalities to existing biocatalysts through engineering of existent enzymes or to discover new enzymes for plant cell wall deconstruction.

2012–2016

- To develop new plants having physical and/or chemical characteristics better suited for transformation into biofuels;
- To develop new biocatalysts and contactors for a more efficient transformation of biomass into biofuels.

2016–2020

- To test plants having a better efficiency towards the use of carbon, nitrogen and water, and a better productivity thanks to the use of nanosystems;
- To develop plants containing some fractionation enzymes inside themselves, with a way of activating the enzymes when the plants are processed for making biofuels.

- **Thermochemical research roadmap**

2008–2015

- Structural model of thermal decomposition of ligno-cellulosic between 50 and 1500°C;
- Model of release of inorganic minor species between 50 and 1500°C;
- Model of nanoscale products formation (sooths).

2012–2020

- Production and test of nanoscale or microscale catalysts and adsorbents operating above water saturation temperature (100°C for 0.1 MPa, 270°C for 7 MPa) and organic minor species condensation temperature (50–450°C according process);
- Use of nanoscale sensors to measure on line parameters (low level of pollutants).

2016–2020

- First biorefineries, coupling between second and third generation processes;
- Test of modified plants residues or micro-seaweeds residues;

Future role of synchrotron radiation and neutron facilities

The use of nanoscale concepts and tools depends on the possibility to conduct investigations at that scale and to incorporate the observations at larger scales. In that respect, it is important to be able to use:

- Micro-imaging and microanalysis of various energies and scales (x-ray, UV and IR) to investigate chemical and structural changes in plant tissues during plant growth or when subjected to environmental changes or industrial processes;
- Time-resolved tools for monitoring biological reactions (like x-ray fluorescence spectroscopy) and for the imaging of enzymes reactions or their interactions with inhibitors;
- Methods for observing interactions of proteins (enzymes) and cell wall components between themselves and at nanosurfaces of heterogenous materials;
- Special attention has to be paid to sample environments to take into account hydration, temperature and mechanical stress, as these variables could greatly influence the properties of biomaterials and their susceptibility to reactions.
- As the structuration and dynamics of water or other solutes has a great influence on biological systems, methods like Deuterium-labelled neutron scattering and spectroscopy would be necessary.

- **Conclusions and European research strategy**

The development of biofuels is necessary to recycle the CO_2 produced by the wide use of energy of each European citizen, at least for a period of fifty to eighty years. The use of agroresources has to be done in a sustainable way and nanoscience and nanotechnology have some potential uses in optimising the production of biomass and its transformation through biological or thermochemical pathways.

Such studies are of course to be connected with progress achieved in the field of nanotechnology, which could provide a special impulse in the fields of food agriculture (often called "green biotechnology"), biological reactions for making pharmaceuticals or chemicals (often called "white biotechnology"), and high performance catalysis in chemical transformations. The aim is to be able to describe and optimise global processes by integration of different length scales and timescales (from nano- to macro-). Within this framework, it is also important for Europe to improve and develop biofuels from lignocellulosic biomass and algae in order to decrease the need on oil in the future, create domestic jobs and better use cultivable lands.

Industrial gas turbines

Metallic construction materials in turbines operate at the limit of their thermal capability and corrosion resistance. Ceramic thermal barrier and corrosion resistant coatings are used to improve the turbine efficiency but are gradually reaching their performance limit.

Nanostructured coatings offer great potential for future applications in gas turbine technology. The main purpose is to develop highly durable and reliable coatings with good mechanical, thermal, and corrosion properties.

The research should develop in the following two directions:

- Prepare, analyse and design tailored coating materials which normally contain multiple layers between the turbine blade and the upper coating;
- Control the in-service performance: the ceramic layers are prone to cracking and spallation from thermomechanical stresses.

Thermal barrier coating on an industrial turbine blade is illustrated in Fig. 5.6.16.

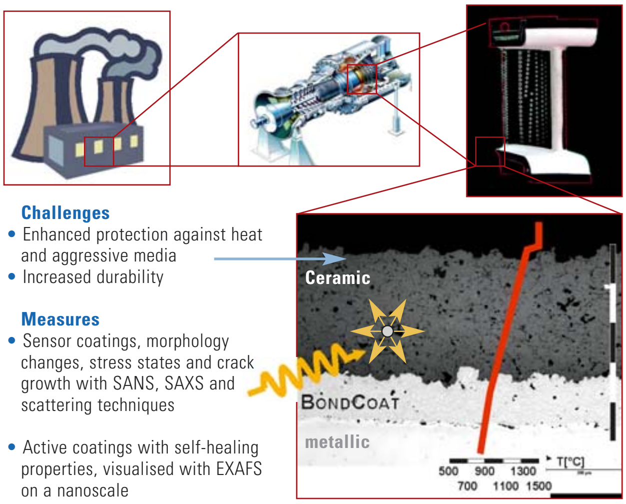

Fig. 5.6.16: Role of synchrotron radiation and neutrons on nanomaterials – thermal barrier coating on an industrial turbine.

Thermal barrier coatings for industrial turbine blade are supposed to provide enhanced protection against heat and aggressive media, and thereby increased durability. To advance the desired properties, diagnostics on the nanometre scale are important. Scattering techniques provide information on stress state and morphology changes. Crack formation can be followed by small angle neutron and x-ray scattering (SANS and SAXS, respectively). Active coatings with self-healing properties are visualised with EXAFS techniques.

Role of synchrotron radiation and neutrons

These analytical techniques are of vital importance in researching the preparation of the coating material, the coating application process and in the performance of coated materials in service.

- Small angle neutron and x-ray scattering (SANS and SAXS) and neutron diffraction techniques detect stresses and morphological changes, crack initiation and growth.
- X-ray Absorption Fine Structure (EXAFS) measurement techniques can visualise local phenomena helping to identify degradation/failure mechanisms and lifetime behaviour.

5.6.3. ENERGY CONVERSION

Nanostructured photovoltaics (Fig. 5.6.17)

Nanomaterials may be used to increase the overall efficiency of PV devices through different concepts. One way is to facilitate the light absorption in the active part by for instance microtexturing the surface, or depositing plasmonic noble metal nanoparticles to couple the light into wave-guided modes. Another possibility is to use nanomaterials to generate photon conversion. Photon conversion processes aim at converting via luminescence the solar spectrum to match the absorption properties of the semiconductor device.

Another concept consists in developing nanostructured semiconductor devices better able to match the solar spectrum. Indeed, nanostructured materials may feature stronger light absorption than their bulk counterparts. Semiconductor quantum dots will allow to design tunable bandgap devices by adapting their size. Silicon nanowires with a diameter of less than 10 nm may also be used to enlarge the bandgap of a PV cell. In all of the above mentioned cases, the interfaces play a crucial role. Being able to probe them by synchrotron radiation is thus of utmost importance.

Role of synchrotron radiation and neutrons

Photo-electron spectroscopy delivers the electronic, energetic and chemical structure of an interface. Effects such as size quantisation lateral band bending and lateral inhomogeneous band offsets will take place.

Photo-electron microscopy (XPEEM) provides structural information, an image of lateral inhomogeneous work function distribution and

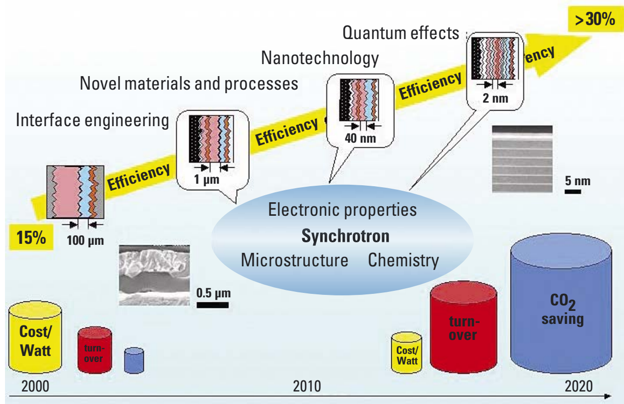

Fig. 5.6.17: Roadmap for thin film photovoltaics: scientific visions and socio-economic benefits.

chemical information (in modern microscopes down to about 20 – 40 nm). The determination of local band gaps, barrier heights and their relation to the local chemical and structural composition is crucial for future development.

X-ray emission microscopy is an important tool for gaining insight into the chemical and morphologic structure of buried interfaces. Working at higher kinetic energies (bulk XPS) will need the development of new types of spectrometres and photo emission beam lines for high resolution studies at photon energies in the 10 keV range. Time-resolved spectroscopy can provide information on the local charge transfer dynamics and to investigate e.g. the excited states of nanoparticles. In order to achieve meaningful results, it is essential to install integrated preparation and analysis systems. Preparation will include wet chemical etching and bath deposition. It will be a challenge to bridge the gap between conventional surface analysis and real life needs.

Conversion

Nanoscale catalysts for the processing of fuels

Catalysts are vital for efficient energy conversion and environmental protection. Nanostructured materials, such as nanoparticles of a catalytically active metal on an oxidic substrate, nanoparticles of gold on a titania substrate, provide an extraordinary opportunity to dramatically improve catalytic performance of: i) energy conversion processes, and ii) decomposition of environmentally hazardous species. The choice of nanomaterials, structural parameters, and the experimental design must be guided by continuously improving fundamental understanding of the structure-function relationships of the nanostructured catalysts materials.

With a view to efficient use of the expensive active component, high dispersion of the nanosized catalyst particles is required. This is particularly true for the expensive noble metal electrocatalysts applied in fuel cells, where particles of 1.5 – 6 nm diametres are applied.Catalytic fuel reforming is essential for approaching the "zero emission" use of fossil fuels. Advanced microreactors feature active coatings with thicknesses in the nanometre range.Drastic increases in the performance of gas separation membranes (providing hydrogen for fuel cells) will critically depend on nanostructuring capabilities.

Materials for solar thermoelectric power generation

Thermoelectric materials are able to convert heat directly into electricity and vice versa. These converters are heat engines without moving parts and show a very good durability and a long lifetime. Like every heat engine the Carnot efficiency is high if the temperature difference between the cold and the hot side is large. High temperature heat (up to 3000 K) can be provided in a clean way with concentrated solar radiation. For the design of high temperature solar energy converters, the development of new materials is required.

Conventional thermoelectrics cannot be applied since they will decompose, melt, oxidise or evaporate under high temperature conditions in air. The only materials which are stable in the focus of a solar concentrator are ceramic materials. Recently, large thermopower was found in ceramics with perovskite related structures. The thermopower in these materials is assumed to be caused by electron spin and electron-electron interactions. To study phase transitions, spin entropy effects, and related spin state transition, high temperature high resolution synchrotron XRD, EXAFS and neutron diffraction data are mandatory. Attempts have been made to produce materials with a temperature stable nanocrystalline structure to lower the heat conduction in the materials.

Numerical calculations have been performed to investigate the interest of introducing silicide nanoparticles into a SiGe alloy to decrease its thermal conductivity at room temperature. The reason why nano-inclusions within an alloy are advantageous in reducing its thermal conductivity is that the heat carrying phonons in the alloy have mean free paths longer than the nano-intrusion spacing, and are thus effectively scattered by the nanoparticles. The use of fine tunable nanoparticles may allow for a lattice thermal conductivity of the order of or smaller then 2 W/m-K if one uses the appropriate silicide particle volume fraction and size. At the same time, electron scattering is not expected to significantly decrease the power factor of the SiGe-based composite, allowing for an increase of the efficiency of the thermoelectric device.

Advanced engineering materials for thermoelectric applications

- Functional materials with enhanced thermoelectric properties and high durability;
- Tailored synthesis methods for structured materials ranging from nano- to macroscale (see Fig. 5.6.18);
- Nanosized and nanoporous powders to thin films and coatings, high quality single crystals of complex metal oxides and nitrides;

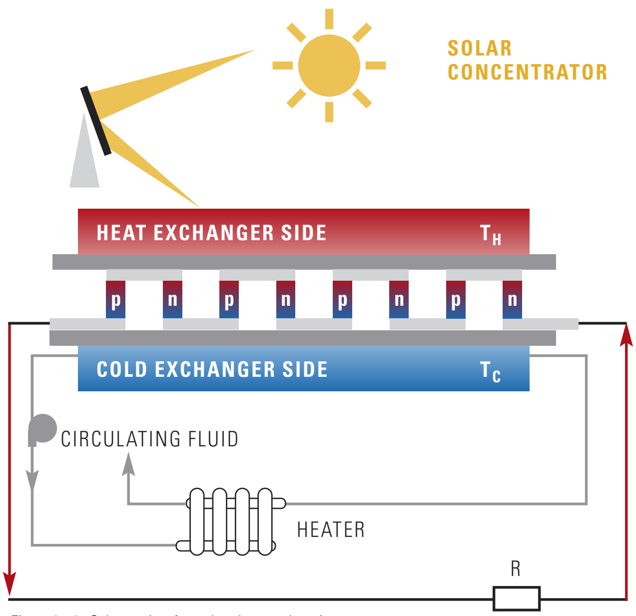

Fig. 5.6.18: Schematic of a solar thermoelectric converter.

- Evaluation of sustainable preparation methods and up-scaling possibilities. Life cycle evaluation of functional materials;
- Analysis and characterisation of the novel materials with standard and advanced methods such as synchrotron, muon- and neutron based techniques;
- Targeted applications are renewable energy technologies.

Role of synchrotron radiation and neutrons

The reproducible synthesis and the development of functional nanostructured materials require a detailed characterisation of the compounds including the description of the structure and composition as well as dynamic processes in the solid.

XAS in solid state chemistry research

- Neutron diffraction techniques are limited to long-range order. They are not element specific and do not give information on local structures;
- For structure determination of materials with crystallite size in the nanometre regime, Transition Electron Microscopy (TEM) and Extended X-ray Absorption Spectroscopy (XAS) methods are applied. XAS in yielding necessary information on:
  - Local structures;
  - The quantitative composition with a low detection limit;
  - The valence state of the ions;

  With EXAFS, inter-atomic distances and coordination numbers of samples with low crystallinity can be determined with great accuracy.

Many perovskite systems are known to undergo structural transitions depending on temperature and/or substitution; i.e., $SrTiO_3$ shows a transition from a cubic to a tetragonal structure below 110 K. Since these transitions are often induced by slight displacements of the anions from their ideal crystallographic positions, they are very hard to detect by x-ray diffraction. With neutron diffraction, the position, site occupation and (isotropic) displacement parameters of the oxygen ions can be determined with high accuracy.

Neutrons in solid state chemistry research

Powder neutron diffraction data offers the unique possibility to distinguish between oxygen and nitrogen, allowing for the detection of a possible O/N ordering on different crystallographic positions. Additionally, neutron diffraction leads to the exact determination of the site occupation as well as the anisotropic displacement parameters of the anions, yielding a deep insight into the crystal structure of perovskite oxynitride phases.

Polymer electrolyte membrane (PEM) fuel cells

Fuel cells are “direct” converters of chemical energy into electrical energy. Low temperature (PEM) fuel cells operate at around 100°C. Research is focused on nanomaterials for membranes and electrodes, with the main objectives being cost efficiency and increased power density.

This fuel cell consists of a proton conductive membrane coated with a very fine layer of catalyst. The R&D needs are summarised as follows:

- Better membrane materials – new proton conductive materials able to transport proton at temperatures higher than 130°C and low humidity;
- Improved membrane materials with low methanol and water crossover for direct methanol fuel cell (DMFC), and high stability;
- Better catalyst materials with better tolerance to CO and higher electrochemical activity;
- Optimised membrane-electrode structures and gas diffusion layers with more effective water management.
- Generate the catalysts at the point where they are the most efficient;
- Develop bio-inspired catalysts to get rid of noble metal catalysts.

PEM fuel cells operating with hydrogen as fuel contain electrodes composed of finely dispersed electrocatalyst particles fixed on a high surface area carbon support. The development of nanosized catalyst particles allows a higher exchange rate due to their intrinsic high surface to volume ratio. It has been demonstrated that the manufacture of in-situ Pt particles at a nanometre size deposited by DLI-MOCVD process has allowed to decrease the amount of noble material by a factor of 3 while keeping the same electrochemical efficiency due to the fact the catalyst particles are formed exactly where they are needed (at the so-called triple point).

Role of synchrotron radiation and neutrons

Scattering methods have already proved to be very helpful in elucidating the membrane structure, distribution of catalysts and understanding proton transport in fuel cells.

Neutron radiography and tomography proved to be extremely effective in visualising important processes in operating fuel cells and stacks, such as the water transport in the channels of the flow field and in the pores of the gas diffusion layers.

Small angle neutron scattering (SANS) yields the structure of ionic clusters in membranes, and reveals their anisotropy and swelling in water. The evolution of water in the cathode of a fuel cell during operation and consequent swelling or changes in the membrane can be visualised.

X-ray scattering (SAXS) and anomalous small angle x-ray scattering (ASAXS) provide information on the distribution of different inorganic components (inorganic additives, catalysts) in the membrane; altering of catalyst particles in operation, by determination of the scattering pattern for specific elements in complex systems (with multi-scattering elements or in the presence of porosity). Particularly informative are the investigation of heavier elements (such as Pt) commonly used as catalyst material or membrane-electrode-assembly components, and the capability of measurements on compact structures.

Increasing the efficiency and affordability of fuel cells requires a better understanding of the molecular-level processes involved in oxidation and reduction at electrodes, catalytic processes, and ion and proton transport, as well as the development of polymer electrolyte-membranes and solid oxide electrolytes. The performance of these components involves several sizes (nm to µm) and time scales which are readily accessible with neutron scattering techniques.

Ceramic high-temperature fuel cells or solid oxide fuel cells (SOFCS)
Solid oxide fuel cells operate in the highest temperature ranges of 700–1000°C. In addition to the use of hydrogen as a fuel, carbon monoxide (CO) is converted into carbon dioxide (CO_2) and desorbed from the hot surface of the SOFC electrodes. In this cycle, the carbon monoxide does not poison the SOFC.

The main drawback of operating a planar SOFC stack with cheap metallic components is degradation (i.e., reduced lifetime) due to chemical and electrochemical reactions at interfaces of different components of the fuel cell system. The membrane-electrode assembly consists of a metallic anode catalyst, an oxygen-conducting ceramic electrolyte layer, and a thin oxide cathode catalyst for oxygen reduction. The fundamental issue is to analyse and to understand the reaction mechanism in order to find new pathways and/or new materials with higher stability, improved lifetime and better performance.

Role of synchrotron radiation and neutrons
Synchrotron based scattering techniques are crucial to follow the surface and the interfacial reactions on a nanoscale level and to record very small, but nonetheless sometimes highly detrimental phase changes during operation. They reveal the oxidation and binding states of elements in the electrode materials, and help to unravel the mechanisms of detrimental performance fading of fuel cells as a consequence of compositional changes.

Performing experiments on operating solid oxide fuel cells requires the development of experimental chambers for an in-situ analysis within the radiation sources. Neutron based methods, in particular SANS, will be instrumental for elucidating the position and location of the light elements hydrogen and oxygen. Synchrotron/SAXS studies provide information on the electrocatalytic reactions that are crucial for the functioning of the fuel cell.

Gas separation membranes
Membranes for molecular separations are expected to play a dominant role in the purification of gases in energy conversion processes. In particular, they are important in various schemes proposed for carbon capture and sequestration (CCS). For post-combustion, efficient separation of CO_2 from an exhaust stream containing large quantities of nitrogen is required. With oxyfuel combustion, efficient techniques for obtaining oxygen from air are desired. In addition, in the advanced pre-combustion schemes that rely on reforming the fuel, the separation of hydrogen from CO_2 is also required.

Some membranes function on the basis of size exclusion (the molecular sieve principle), while others make use of specific molecular interactions between the permeating compounds and the membrane and function on the basis of solid state diffusion.

The most important membrane materials under development are:
- Dense noble metal membranes (hydrogen separation);
- Dense ceramic proton conducting membranes (hydrogen separation);
- Dense ceramic oxygen conducting membranes (oxygen separation);
- Dense ceramic mixed conducting membranes (oxygen or hydrogen separation);
- Microporous ceramic membranes (several molecular separations).

Since the amounts of gases processed in power plants are very high, the membranes need to have – besides high gas selectivity – a high

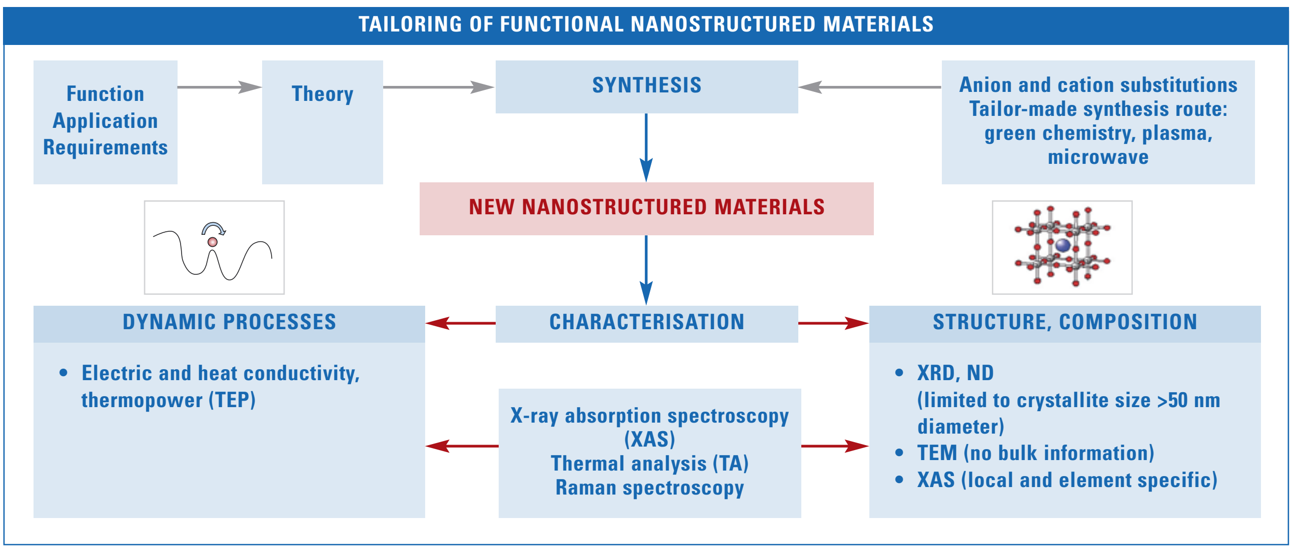

Fig. 5.6.19: Syntheses of nanostructured materials.

gas permeation capability. These requirements can be fulfilled by extremely thin layers with either a well-defined microporosity or high atomic/ionic (/electronic) conductivities. Therefore, the preparation of these layers is a very challenging task. Nanoporous materials can be extremely useful in separation because of their ability to recognise and discriminate between molecules.

Role of synchrotron radiation and neutrons

Experimentation in-situ is of utmost importance to optimise the preparation processes and the properties of the layers.

Synchrotron radiation (SAXS) allows analysis of nanoparticles with regard to their morphology, which determines the micro- and nanostructural properties of the membranes. This is especially the case for sol/gel derived microporous membranes where the properties strongly depend on the size and form of the primary species (oligomers).

Neutron scattering techniques are extremely useful because of the completely different distribution of scattering cross sections, in comparison with x-rays. This enables the determination of the position of light elements, (e.g., H and O), in the presence of heavy metals, (e.g. Fe, Co, Ba, and Ce in perovskites). In addition, it provides an essential insight into the defect chemistry of these materials.

EXAFS techniques are ideal for research on noble metal membranes for hydrogen separation to unravel the local structure (coordination sphere) of the predominant metal and the alloying elements.
Reflectometry gives valuable information on layer thickness and compositional gradients.

5.6.4. ENERGY STORAGE AND TRANSPORTATION

In spite of being widely used, today's batteries/accumulators and capacitors still offer the potential for substantial increases in specifications. The compromise between production cost and device performance parameters like capacity, charge and discharge behaviour, and durability is a challenge for industry.

Micro- and nanomaterials have a key role to play as they offer the possibility of improving all aspects of battery performance, i.e. higher capacity electrodes with higher electronic conductivities, mechanical properties, low toxicity, and electrolytes with higher ionic conductivities, chemical stability and low toxicity.

Nanomaterials for Li-ion batteries: the general advantages of nanostructured active electrode materials are as follows:

i) A larger electrode/electrolyte contact area leading to higher charge/discharge rates;
ii) Short path lengths for both Li-ion and electronic transport permitting the use of low ionic and low electronic conductors;
iii) An improved mechanical resistance of particles related to volume changes generated by insertion/extraction processes of H^+ and Li^+ ions.

Moreover, it has been recently demonstrated that materials that were thought electrochemically inactive in bulk form can present improved electrochemical performance at the nanoscale. A last possibility for improved battery performance is to manufacture composite nanopowders in a core-shell structure with a core made of low electronic conducting material and a shell made of high electronic conductors such as C to get a good electronic percolation in the electrode.

The electrochemical processes at the electrodes and the electrolyte are mostly correlated to the atomic scale at surfaces, of phase boundaries and in the bulk. Therefore, characterisation methods at the nanoscale are essential. To analyse structure-property correlations in active electrode materials, it is necessary to follow structural changes during charging and discharging processes. This implies in-situ measuring techniques, i.e. integration of electrochemical cells in the sample holder for diffraction experiments. The need for containment of such electrochemical cells implies either high intensity radiation sources (synchrotron radiation) or low absorbing radiation for scattering experiments (neutrons).

Accumulators (Fig. 5.6.20)

The structure as well as the chemistry of the active material can influence the maximum specific capacitance and the ionic and electronic conductivity. The charge/discharge cycling is responsible for phase transitions and durability problems of intercalation compounds. The same holds for the volume breathing of the device due to shifts in lattice constants which can be analysed by diffraction methods. Order/disorder phenomena in multinary compounds and the stability during cycling are of prime interest.

Role of synchrotron radiation and neutrons

The development of optimised in-situ electrochemical cells for diffraction experiments using intense synchrotron radiation and neutron beams is a quantum step in being able to look at structural aspects of the active electrode materials in real working conditions. These structural aspects i.e. phase transitions, Li-intercalation and ageing, have to be correlated to the battery device performance in order to understand the mechanisms and finally develop devices of improved quality. Grazing incidence techniques, such as surface XRD at high brightness synchrotron sources, are crucial to elucidate the structure of the thin active surface layers.

This is also true for XAS studies which are very well appropriate for the study of local structural and electronic changes induced by the functioning of the battery. The next step in the use of this technique will consist in performing time-resolved techniques (Quick XAS and Dispersive XAS) in order to characterise the battery materials during functioning. The now available micrometre spatial resolution will also allow considering the impact of inhomogeniety on the battery performances. One should also consider the use of quasi-elastic neutron scattering, QENS, at very low energies and deep inelastic scattering, DINS, at the extreme high-energy end. It may be possible to study Li (and

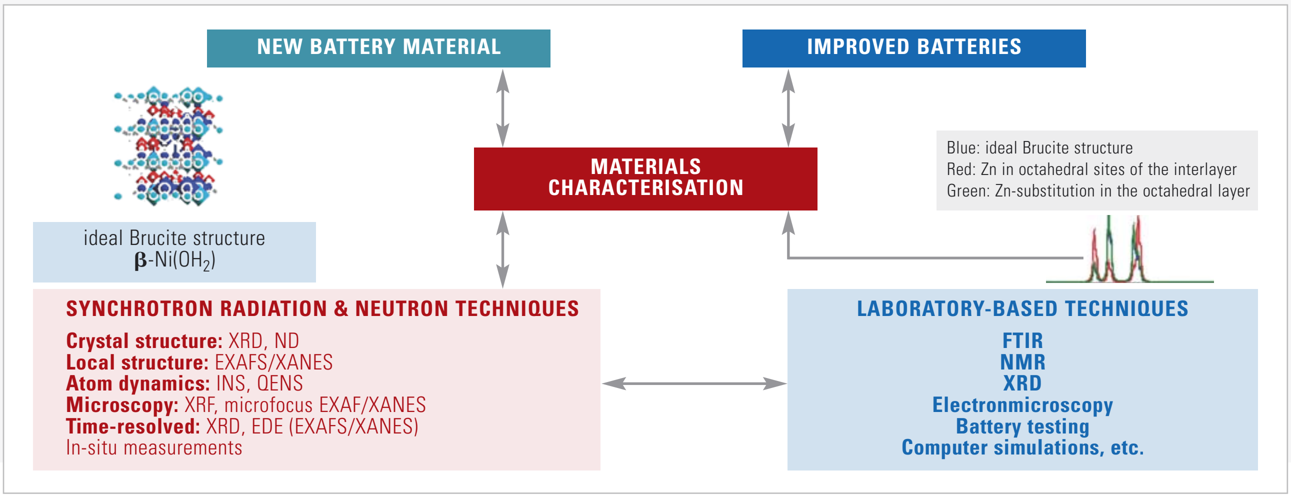

Fig. 5.6.20: Schematic diagramme showing the role of synchrotron radiation and neutrons for nanomaterials developments in batteries.

other ions) transport in a non-hydrogenous system using QENS. More novel would be the use of DINS to directly probe the momentum distribution associated with the Li ions present – in other words to study the potential in which the Li ions move.

Super capacitors (Fig. 5.6.21)
Double layer capacitors or super capacitors play an important role in applications of energy storage, where high power either in charging or discharging steps is demanded (e.g., acceleration and deceleration of vehicles). The electric charge is stored in an ionic layer formed at the interface between each of the two electrodes and a common electrolyte. Therefore, the extension of the interface plays an important role. In addition, a principle task of super capacitor electrode characterisation is the estimation of its porous structure.

Role of synchrotron radiation and neutrons

The dimensions of the building units of active carbon suggest small angle scattering methods (SANS) for structural characterisation. The differences of the electron densities in the bulk and the porous volumes are the cause of small angle scattering intensities and, therefore, the key to structural information. As for the battery electrode materials, in-situ measurements on working devices will give information of the electron density shifts due to ion ordering in the electrodes. The challenge will be the structural interpretation of scattering intensities and finally correlation to the device performance.

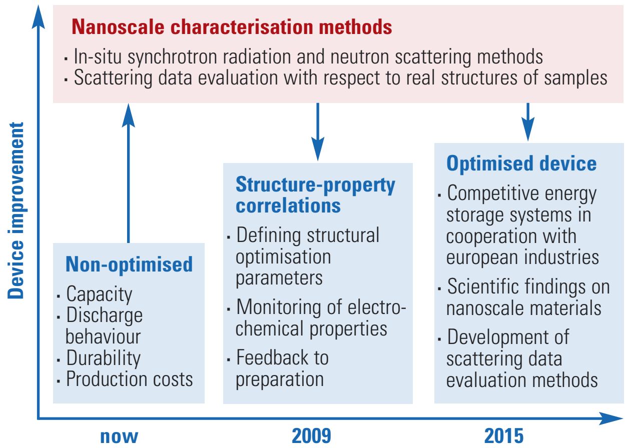

Fig. 5.6.21: Roadmap for accumulators and super capacitors.

Key targets in electrochemical research with synchrotron radiation and neutrons

- Tailoring of new nanomaterials and the development of nanomaterials-processing techniques for battery application;
- Understanding the degradation mechanisms during experiments and in service operation; a number of electrodes composed of micro- and nanomaterials show poor recyclability due to structural and chemical changes (in oxidation state); degradation of thin film batteries;
- Study of surfaces and interfaces, especially to gain insight into the near-surface reaction mechanisms;
- Development of in-situ methods for the investigation of battery materials under operating conditions and the construction of in-situ cells for operation at x-ray and neutron sources;
- Improvement of electrolytes by additions of micro- and nanoinert fillers, such as silica, alumina;
- Optimising nanomaterials processing techniques, mastering service lifetime requirements, and subsequent optimisation in battery applications.

Understanding the role of micro- and nanomaterials and the subsequent optimisation in battery applications requires detailed chemical and physical characterisation. In this respect synchrotron radiation and neutron techniques offer the most universal methods.

Nanoscale materials for hydrogen storage

The major bottleneck for commercialising fuel cell vehicles is onboard hydrogen storage. Hydrogen exhibits the greatest higher heating value (39.4 kWh/kg) of all chemical fuels. The critical point of hydrogen is at a temperature of 33 K. Therefore, the dense storage of hydrogen is a materials challenge and the interaction between hydrogen and the surface and bulk of materials is crucial. Hydrogen can be stored by six different methods and phenomena:

- High pressure gas cylinders (up to 800 bar);
- Liquid hydrogen in cryogenic tanks (at 21 K);
- Adsorbed hydrogen on materials with a large specific surface area (at T< 100 K);
- Absorbed on interstitial sites in a host metal (at ambient pressure and temperature);
- Chemically bound in covalent and ionic compounds (at ambient pressure);
- Oxidation of reactive metals e.g. Li, Na, with water.

The presently available systems are high pressure tanks or liquefied hydrogen in cryogenic vessels, which both possess severe disadvantages, e.g. large size and potentially low consumer acceptance concerning safety aspects. Storage of hydrogen in light-weight solids could be the solution to this problem. During the last few years, novel nanoscale materials which show new kinetics of adsorption and desorption as well as new thermodynamic properties, have been synthesised for hydrogen storage (see Fig. 5.6.22).

For hydrogen physisorption, new nanoscale materials with high specific surface area are needed. Needed materials include carbon nanostructures and novel nanostructured materials with extremely large specific surface areas, such as metal-organic frameworks (MOF's).

Carbon nanostructures and other novel nanostructured materials with an extremely large specific surface area possess a high potential for hydrogen storage by physisorption at lower temperatures.

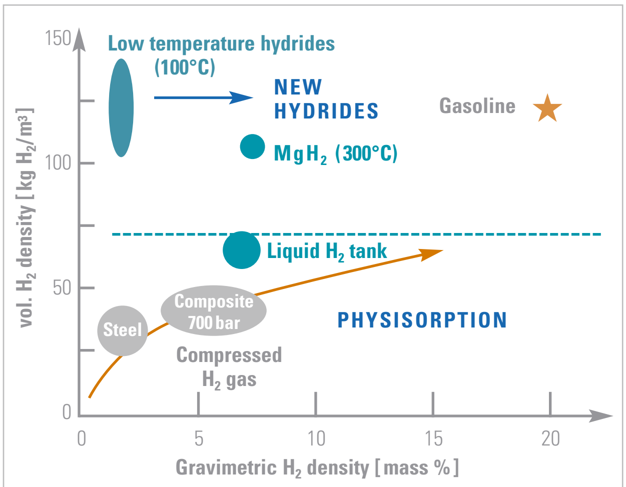

Fig. 5.6.22: Overview of nanomaterials in hydrogen storage.

Nanostructured magnesium hydride with added oxide particles exhibits drastically improved absorption and desorption kinetics of hydrogen. Complex hydrides can be reversibly operated in a temperature range required for fuel cells by applying nanoclusters of catalyst. Therefore, the goal and vision of future studies on nanoscale materials is to understand the nature of the processes occurring on the nanoscale and to be able to design optimised hydrogen storage materials for technical applications (see Fig. 5.6.23).

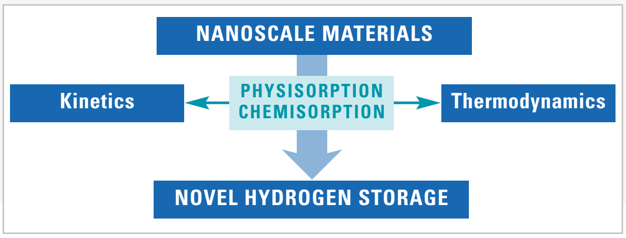

Fig. 5.6.23: Future challenge in fundamental research role of nanomaterials for hydrogen storage.

Presently, sluggish reaction kinetics for adsorption and desorption of light metal hydrides limit the loading times at fuel stations, the actual availability of the necessary volumes during application and the temperature range feasible for customer safety and "wellness". The most promising route to overcome these deficiencies is the development of suitable nanocrystalline composites (Mg-hydrides and metal oxide catalysts).

The greatest values for the volumetric densities of hydrogen are found in metal hydrides. The crystal and electronic structure of the host metal define the interaction with hydrogen. The surface of the solids plays a crucial role for the stability of the hydride and the kinetics of the hydrogen sorption. Therefore, nanostructured materials allow tailoring the properties of hydrides.

The need for neutrons and the support of synchrotron radiation to study nanomaterials for hydrogen

To characterise the materials and processes involved in hydrogen production, storage, and use, one needs information about the following:

- Atomic- and molecular-level information on structure;
- Hydrogen diffusion;
- Interatomic interactions;
- Nanoscale and macroscopic morphologies.

Neutron scattering provides unique capabilities for giving this basic information and is vital for investigations related to catalysis, membranes, proton conductors, hydrogen storage materials, and other materials and processes related to hydrogen production, storage, and use.

Neutrons can identify the presence of hydrogen atoms in the structures of alanates used for hydrogen storage. Structural characterisation using x-rays cannot reveal the site of hydrogen incorporation, which is critical to a fundamental understanding of the mechanisms of hydrogen storage.

Neutrons have a unique ability to distinguish hydrogen from deuterium, allowing isotope substitution to be used to provide additional insight into the structure of materials and into the interactions occurring between hydrogen and these materials. Neutron-based techniques have the potential to study nanomaterials and chemical processes under realistic conditions, rather than under the high-vacuum or other controlled and environmental conditions.

The intense flux of the spallation neutron source will permit neutron diffraction to determine hydrogen positions accurately and dynamically. Inelastic spectrometres allow researchers to examine diffusion processes on an atomistic level and relate them to structure.

Understanding this relationship is a vital step to developing better, more affordable nanomaterials, such as membranes for selective purification of hydrogen. Similar techniques can be applied to determining diffusion paths in promising proton and ion conductors. Single-pulse determinations will allow in-situ measurements to be made in real-time during charging/discharging cycles in hydrogen storage materials and as a function of external parameters, such as pressure and temperature.

Synchrotron radiation is wellsuited as a complementary technique to monitor the lattice response, defect creation and in-situ studies of fast reactions.

Systematic neutron and synchrotron radiation studies of new nanoscale materials under cyclic hydrogen charging and discharging have to be undertaken in order to provide a solid database for potential applications. This includes the kinetics of charging and discharging (lattice response) and the monitoring of lattice damage and materials degradation under cyclic loading.

5.6.5. ENERGY SAVING

Tailoring of interfaces to manipulate energy carriers

Engineered nanostructures at interfaces have great potentials in improving the efficiency of energy systems and components i.e. low-power electronics, efficient use in lighting, energy harvesting. The challenge is to tailor the interface functionality at the nanometre length scale for:

- Electron transport (electrical transmission, losses, small devices);
- Electron and phonon transport (thermo-electrics);
- Photon collection and electron and exciton transport (photo-voltaic);
- Electron and hole recombination (lighting).

The targets of controlling the energy transport across nanoscale interfaces are crucial to advances in energy use and energy harvesting and demand for research in:

- Syntheses of novel interface shapes/structures: using a wide range of nanomaterials and chemical combinations; exploiting a diverse array of methods: top-down lithography, self-assembling materials growth, wet-chemical processing, biological assembly and combinations of these synthesis methods;
- Developing and using experimental techniques for nanoscale characterisation to relate structure to function;
- Investigation of electron transport phenomena at the nanoscale (classical descriptions of tunnelling, confined dimensionality are inadequate – nanoscale devices will be dominated by surfaces!).

Study of new phenomena and properties at the nanoscale

Nanomaterials have unique structures and behaviour that cannot be extrapolated from our understanding of bulk materials. The challenge is how to make nanomaterials science useful at the macroscopic scale. The overarching research challenge that we face is establishing the physical and chemical principles that determine the functionality that emerges at nanometre length scales, and exploiting this functionality for improving energy technology:

- Effects of quantum confinement;
- The enhancement of interfacial free energies over bulk free energies;
- The importance of surface states;
- The mechanical properties of nanostructures – multiple length scale simulation of crack propagation;
- Fluid-flow in nanoporous structures.

Research is needed into ultrahigh strength, lightweight nanophase structural materials, e.g., nanocomposite ceramics, with enhanced mechanical properties. Oxide Dispersed Steels (materials with dispersed oxide nanoparticles) and infiltrated ceramic are developed for high temperature resistant materials, which are of importance for achieving higher efficiencies in combustion devices, high temperature solar technologies, and advanced nuclear reactors.

Nanomaterials in large-scale production:
"new, cost-competitive, reliable, long lifetime"

The ultimate goal – to meet the energy technology target – is to manufacture nanomaterials in large quantities and to construct components at a practical manufacturing level in a controlled manner. The processing of nanomaterials involves the following challenges:

Quality synthesising promising nanomaterials of high purity, free from defects, of reliable and reproducible properties with standards reference;

Quantity developing and optimising processing methods for economical, large-scale production of nanomaterials; this requires scalability and low-cost methods for producing large scale production of nanomaterials;

Variety requiring research and development of methods to efficiently explore and expand the library of "building blocks" of enhanced nanomaterial properties that are potentially available for use;

Integrated design developing methods that are compatible with the concurrent assembly of nanomaterials into systems/architectures and/or components that permit their greatly enhanced properties to be expressed at the macroscale. This also implies joining, machining and non-destructive techniques of nano- with nano- and/or macro-materials.

5.7. NANOTECHNOLOGY IN THE PROCESSING INDUSTRY

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[Affiliations chapter 12]

All stages of manufacturing, from materials production, through materials processing, device/component fabrication, and assembly to the treatment of finished products, rely on a sound understanding of materials behaviour and how process conditions can influence final performance. Intelligent nanomicrostructural control is the key to adding value and obtaining optimal properties. Processing encompasses everything from the chemical formation of polymers, through casting of metal alloys and forming them into components, to surface engineering of the final product, as shown in Fig. 5.7.1.

Fig. 5.7.1: Materials production and processing.

Whilst significant progress has been made in the characterisation and improvement of conventional techniques in the traditional manufacturing disciplines, the opportunities for step-jump improvements offered by nanomaterials require a new level of sophistication and understanding in the application and extension of existing methods to these new classes of materials. Many conventional processing methods will need to be refined or replaced since they disrupt or destroy the structures which have been deliberately engineered at the nanoscale.

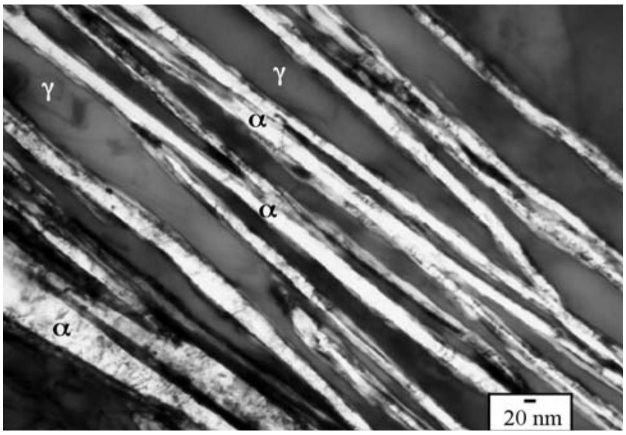

Fig. 5.7.2: Plates of bainite only 20–40 nm thick are dispersed in stable carbon-enriched austenite which, with its face-centred cubic lattice, buffers the propagation of cracks.

Nanotechnologies are not just for small-scale specialist applications. There are significant possibilities in the development of relatively 'conventional' materials. The $Fe_{1.5}Si_2Mn_1C$ wt% steel illustrates how knowledge of thermodynamics and diffusion can be put to good effect to deliver nanostructured materials by the tonne. Plates of bainite only 20–40 nm thick are dispersed in stable carbon-enriched austenite which, with its face-centred cubic lattice, buffers the propagation of cracks (see Fig 5.7.2). Much of the strength and hardness of the microstructure comes from the very small thickness of the bainite plates. Of the total strength of 2500 MPa, some 1600 MPa – nearly two-thirds of the total – has been attributed solely to the nanostructure of the plates. This shows the great opportunities for the improvement of bulk steel without the use of expensive alloying elements. Hence, nanomaterials can have a major impact in traditional "heavy" industry as well as the formation of new manufacturing technologies and processes.

In order for industry to meet future requirements of properties, cost and performance, it is necessary to understand the fundamental mechanisms of processing by in-situ analysis of reactions, phase transformations, treatments and processes. By combining in-situ synchrotron, neutron, SEM and TEM studies with the more traditional ex-situ studies, improved understanding can be used to refine existing models of materials behaviour as well as generating new models of new phenomena. In the long term, this will ensure more precise and efficient production of new materials with improved properties.

Completely new manufacturing processes need to be developed that will not have macroscale analogues. Self-assembly is an example of the kind of typical manufacturing method which is used in nature to assemble various molecules and structures. Imitating these strategies and creating novel molecules with the ability to self-assemble into supramolecular assemblies is an important technique in nanotechnology. In self-assembly (see Fig. 5.7.3), the final (desired) structure is "encoded" in the shape and properties of the molecules that are used, as compared to traditional techniques, such as lithography, where the desired final structure must be carved out from a larger block of matter.

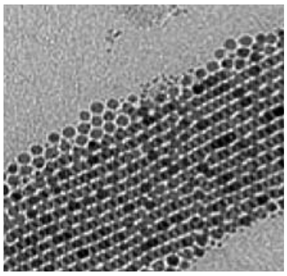

Fig. 5.7.3: Magnetically self-assembled array of Co nanocrystals.

Nanostructures

The main fabrication routes for nano-objects (colloids, rods and platelets) will still be chemical synthesis and flame pyrolysis. As a "top-down" process, many concepts will be derived from microelectronic processing i.e. lithography and metal deposition (PVD, CVD and electroplating for the formation of metals and alloys). Electrodeposition, which is a standard process in microelectronics nowadays, has also been employed extensively for the fabrication of nanocrystalline bulk metals. On an even larger macroscopic scale, severe plastic deformation of metals can be used for the formation of nanocrystalline grain structures, especially if care is taken with the strain rate and processing temperature. All of the novel fabrication routes for nanomaterials suffer from the difficulties in upscaling potential. Here, new processing routes will have to be found.

The key to intelligent processing is a means of monitoring the structural changes in-situ in real-time. This is where the capabilities of neutron and synchrotron x-ray sources become essential. They can deliver unique information for the optimisation of new processing methods, using dedicated prototype production facilities for the monitoring of in-situ experiments. New approaches and techniques can be trialled with small-scale prototype investigations at the facilities, radically accelerating the process development cycle. The results could then be used to inform the development, construction and operation of new plants to exploit better understanding and ensure the delivery of the required properties from a range of nanomaterials and applications. In this manner, process development can be turned from 'black art' into informed scientific development.

Modelled design

Understanding of scaling laws is the key to understanding the properties of nanomaterials. Research should focus on novel nanoscale-induced properties, but also on how they can be tuned by length scale variation. In many cases, the smallest constituents will not necessarily yield the best properties, but rather the ones with the optimal length scale, which in some instances may exceed the nanoscale. Surface effects, for instance, will also change the phase stability at small scales and result in novel thermodynamically stable phases. These will also result in new properties.

Our ability to invent new nanoscale materials and devices will be dependent upon, and open up new opportunities for, atomistic modelling as the representative volume elements become smaller and smaller. In this case, the length scales can be modelled correctly and the challenge will lie in improving models to also include the relevant timescale. Again, basic underpinning physics information such as diffusion and self-diffusion coefficients will only be obtainable by neutron scattering.

Impact of neutron and synchrotron radiation techniques in the optimisation of manufacturing processes

For the successful improvement in process technologies to deliver future competitive products based on nanomaterials and nanodevices, there are several important and interdependent steps which need to be addressed:

- The ability to develop and operate mock-up or prototype processing facilities at neutron and synchrotron x-ray sources;
- Increased flux to allow for the study of structural changes during processing at faster frame rates;
- Development of the necessary sample environments to support in-situ process experiments and the handling of large samples;
- Provision of software support for the design, control and analysis of experiments;
- Materials scientists – not just instrument scientists – supporting beam lines.

5.7.1. METALLURGY

Nanometallurgy has recently been described as the capability to manipulate metals on the atomic scale. In broader terms, one could define it as the science and technology of metals with new properties caused by nanostructuring and alloying at the nanoscale. The nanodimension may either be external (quantum dots, wires and thin films, nanoplatelets and colloids) or internal (nanocrystalline metals, nanoporous metals or metal-based nanocomposites). Traditionally, nanoscale features have been used to change the properties of metals for decades (e.g., powder metallurgy, oxide dispersion strengthening) or in some instances for centuries (carbon nanotubes in ancient damascene swords). The term nanometallurgy is reserved for the creation of new properties that rely on the deliberate use of nanoscale

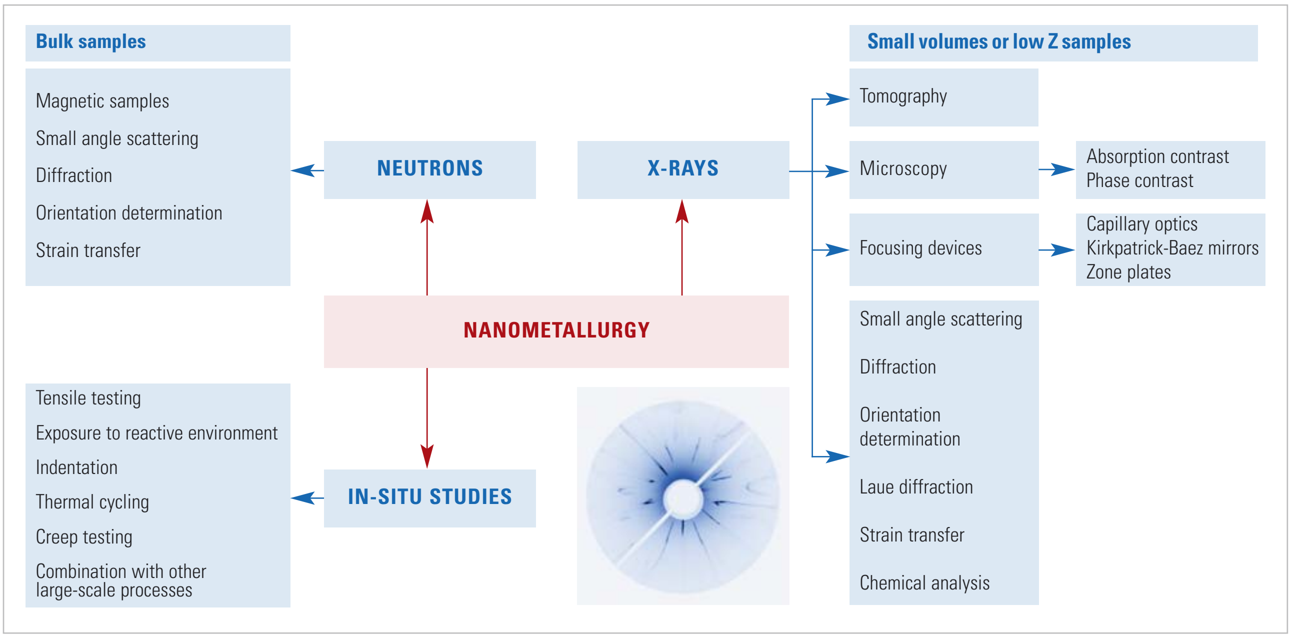

Fig. 5.7.4: Importance of synchrotron radiation and neutrons in the development of the "nanometallurgy".

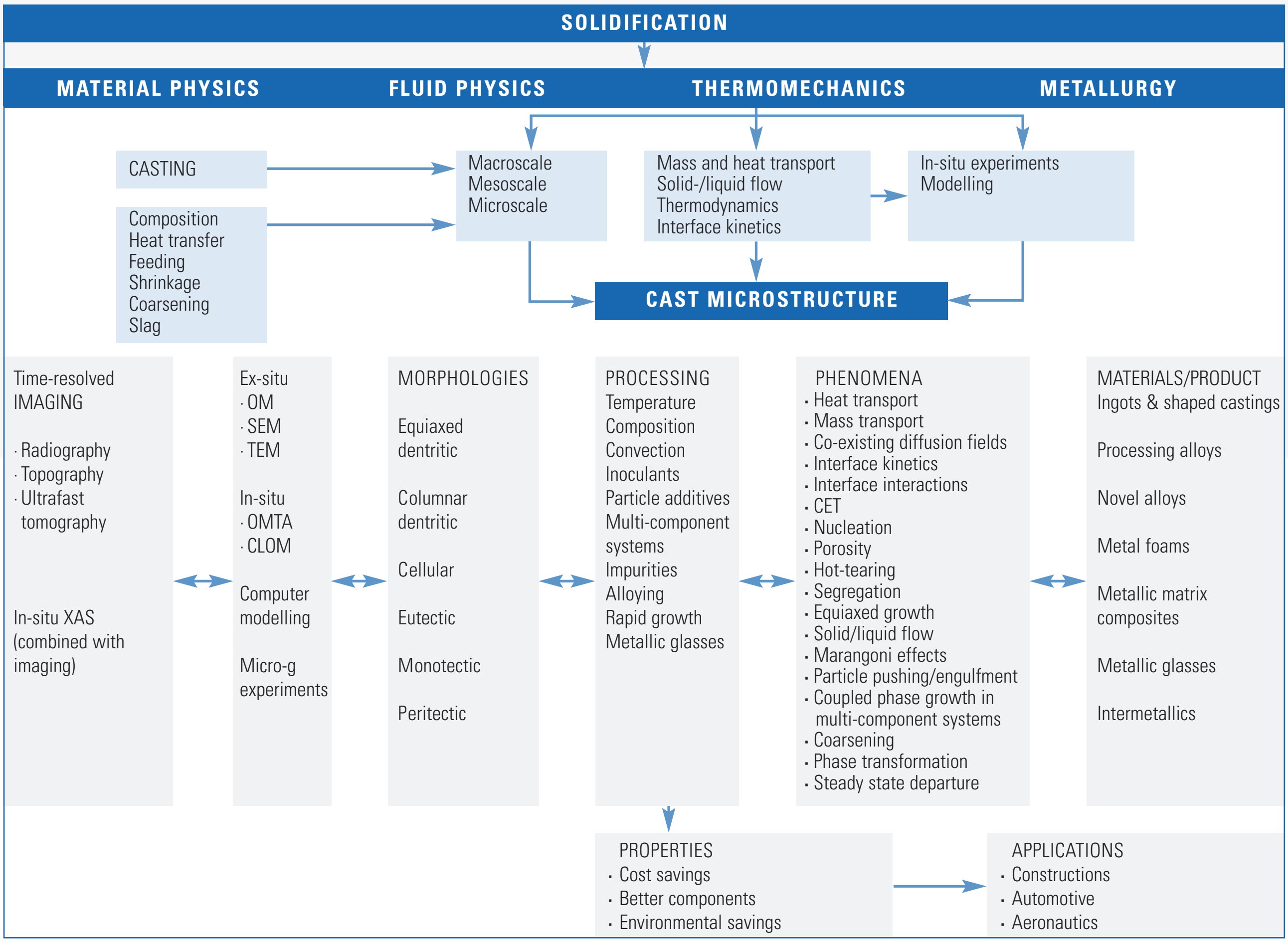

Fig. 5.7.5: New developments in the "solidification" process.

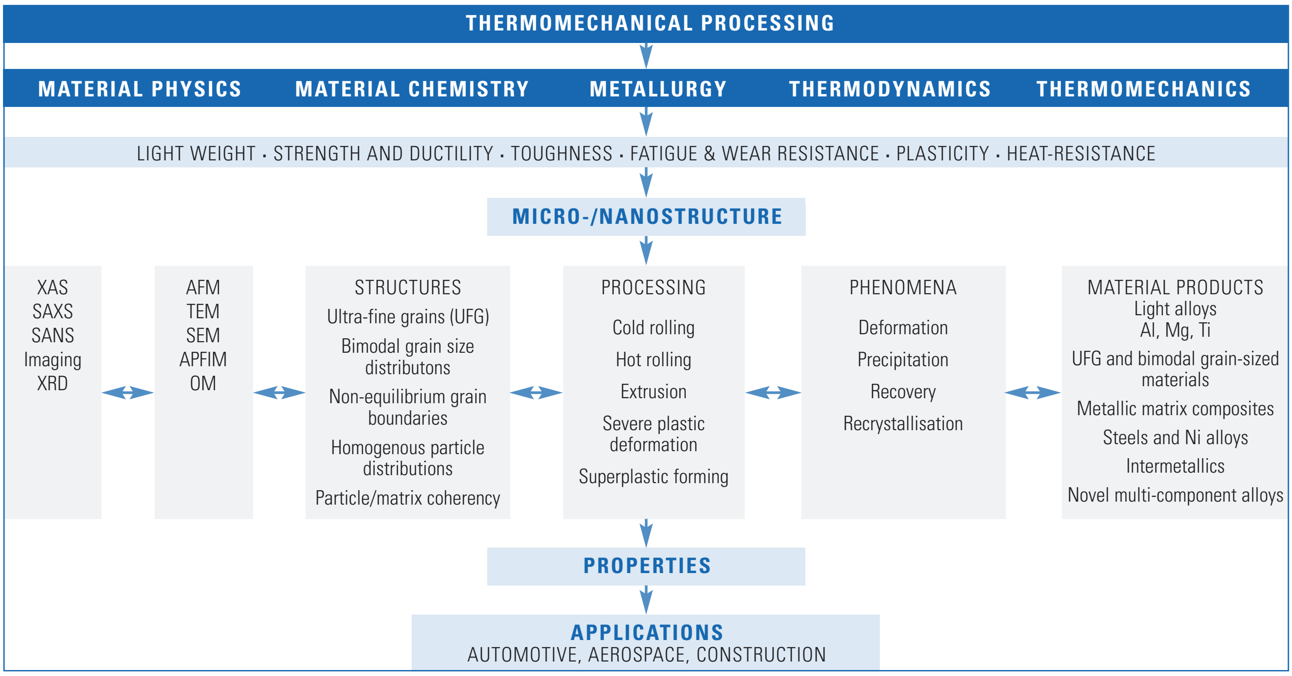

Fig. 5.7.6: Thermomechanical processing for metallic nanostructures.

features and alloying. Nanostructures can be introduced during solidification or by secondary processing (see Fig. 5.7.4).

Experiments can be performed to monitor processes such as solidification or joining in real-time, utilising the high flux of modern instruments to obtain the necessary high time resolution. While numerical computer modelling for simulations of solidification has advanced considerably over the last couple of decades, provision of new experimental data to guide theory and modelling and assist in their refinement has fallen behind. Recent improvements in x-ray detectors, combined with the inherent brightness and collimation offered at third generation synchrotron sources has opened the way for both x-ray radiography and tomography investigations of solidification phenomena (see Fig. 5.7.5).

Secondary processes like forming are accompanied by changes on the micro- and nanostructural scale, which greatly influence the properties of the final product. To ensure high quality, identifying, controlling and quantifying the various reactions, phase changes, and structure development occurring on the nano- and microstructural level will be essential to maintain competitiveness and deliver optimised properties (see Fig. 5.7.6).

Why neutron and synchrotron instruments?

Neutron and synchrotron sources are particularly relevant because they can provide the following: i) phase evolution information by diffraction, ii) nanostructural scale and morphology distributions by SANS/SAXS, and iii) fine-scale imaging by tomography. All of the above occur in a realistic process environment, approaching real-time in a non-destructive fashion. With bulk scale nanostructured materials appearing, neutrons are needed for nanostructured samples whose macroscopic dimensions render them x-ray opaque. Synchrotron sources, on the other hand, offer the ability to study the fast transformations in real-time. In-situ experiments (mechanical deformation, heat treatment, current exposure, chemical treatment) will become more and more important to develop a fundamental understanding of the mechanisms acting at the nanoscale and to control them to our advantage. These in-situ experiments require a collaboration between large-scale facilities and analytical facilities, which are currently only available in the laboratory environment such as scanning electron microscopy, Raman microspectroscopy and many others (see Fig. 5.7.7). The transmission electron microscope with all its different modes of operation (STEM, tomography, EDX, high resolution, EELS) will be a key tool for nanometallurgy, though TEM are restricted to very thin sections and surface observation. However, microfocused synchro-

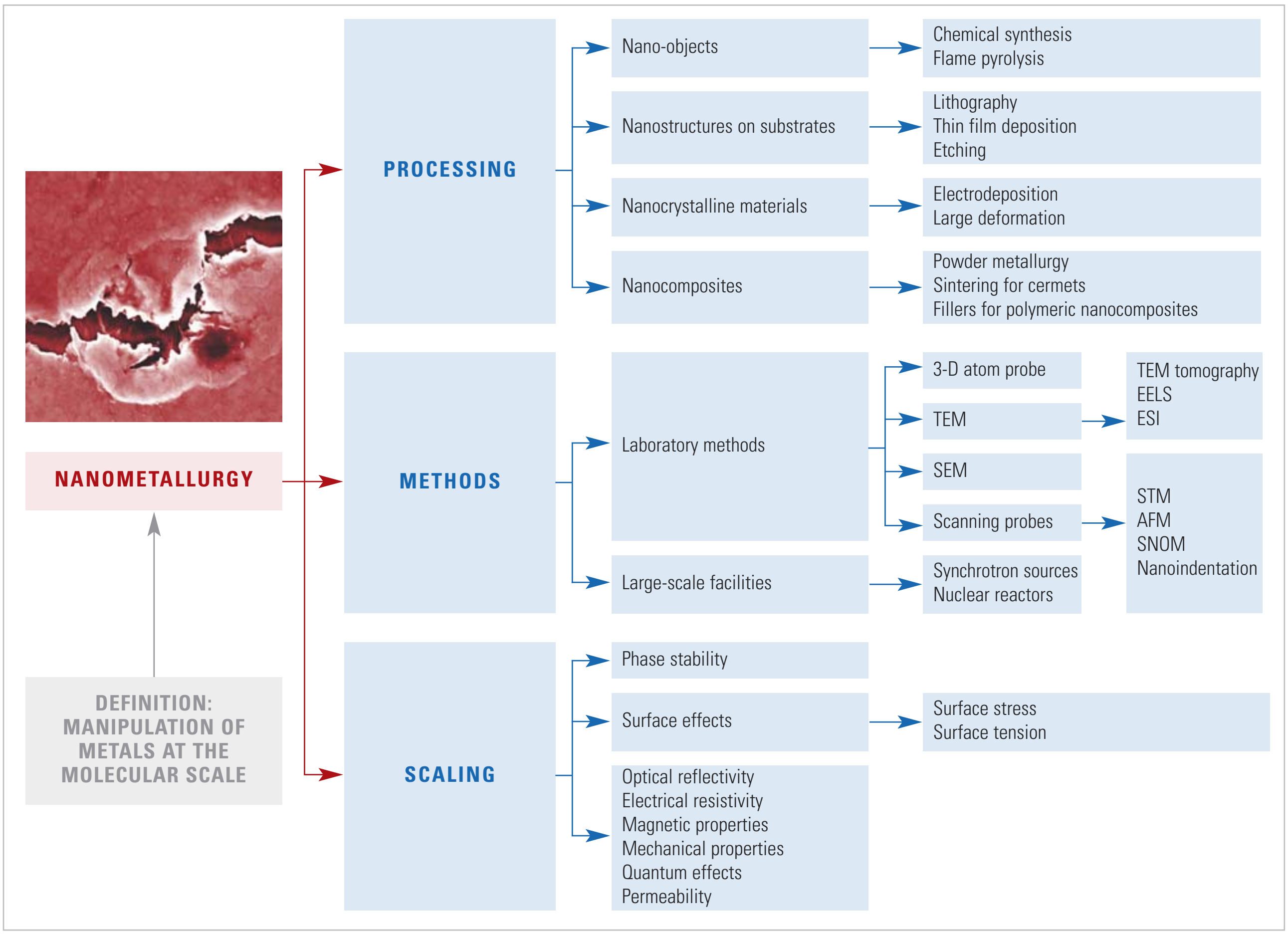

Fig. 5.7.7: Manipulation of metallic materials at the molecular scale.

tron probes are beginning to release us from these traditional constraints. Scanning probe methods will also be used for materials with externally small dimensions. The recent commercialisation of 3-D atom probes with their extremely high spatial and compositional resolution will become a standard tool for nanometallurgy.

Bulk processes

One of the key challenges of nanometallurgy will be to upscale the research-oriented processes to become industrially relevant. This will also require the development of new processing routes that are economically viable. The upscaling will have to be achieved in number (for nano-objects) and in the external material dimension for nanostructured materials. A combination of traditional metallurgy with novel alloying concepts will be the key to success in this aspect and will rely on exploiting our understanding of equilibrium and non-equilibrium processes. Key to obtaining many nanostructures will be control over nucleation, phase stability and phase transformation either in the liquid or solid states. For bulk materials to be processed, it is crucial that process windows are established at practical temperatures and cooling rates. Here, neutron and synchrotron methods can provide much basic information regarding transformation rates, phase diagrammes, diffusion coefficients and nucleation events, enabling process optimisation driven by the understanding of science and the engineering fundamentals. Nanostructured bainitic steels (Fig. 5.7.2) provide a good example of how exploitation of phase diagramme modelling can be used to develop alloys which can be strengthened by extremely fine nanostructures cooled at modest rates. In-situ diffraction provides information about the transformation kinetics and variant selection.

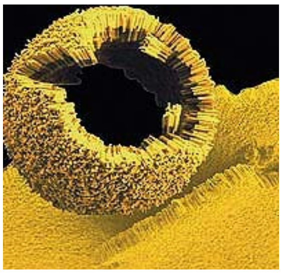

Fig. 5.7.8: Self-assembly of gold-polymer nanorods results in a curved structure.

5.7.2. CERAMICS

This area is covered in detail in the chapter on structural nanomaterials (see chapter 3.3). In essence, it is relatively easy but very expensive to obtain nanopowders. New cheaper nanopowder production methods are required, but equally as important: we need to learn ways to form products without losing the nanostructure of the constituent powder. Very tight control of temperature and pressure is required during the power process if grain growth is not to erase the nanostructuring. Without size information provided by neutron/synchrotron scattering, it will be very difficult to obtain the best processing parameters (see Figs. 5.7.8 and 5.7.9).

Nature has developed self-assembly processes capable of manufacturing structures of tremendously rich scale levels; including shells, bone and other supporting structures. We need to develop chemical or self-assembly methods to replicate these tough structures.

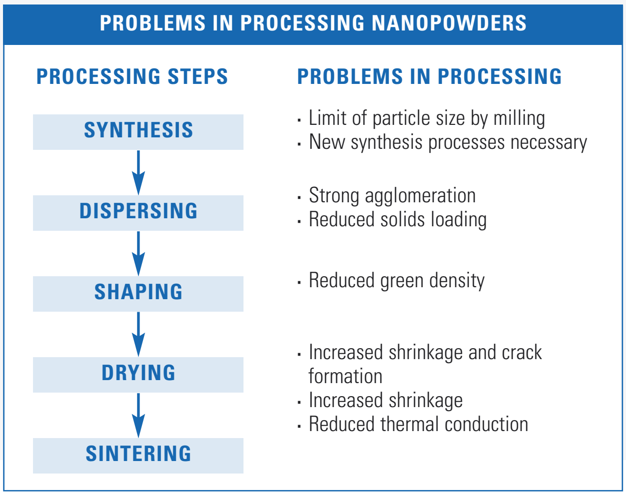

Fig. 5.7.9: Problems in processing nanopowders.

5.7.3. POLYMERS AND COMPOSITES

Polymer blends can be manufactured with extremely fine microstructures if the rheology of the process and the thermodynamics of mixing are well understood. A new chaotic advection-based process has been developed where plastic extrusions of various forms (e.g., film, pipe, sheet, etc.) can be produced with a variety of blend morphologies in continuous lengths. Essentially, morphology is selectable online by control of chaotic advection and other parameters such that no equipment modifications are required. In Fig. 5.7.10 an example is shown of a novel blend containing thousands of internal sub-micron layers. The thicknesses and number of layers are selectable by process control using "smart" blending devices. Fibrous, interpenetrating, platelet, percolating, and droplet morphologies are examples of other blend morphologies that have been formed).

Nanocomposites (Fig. 5.7.11): New combinations of materials properties will be provided by new phases, alloys with a large number of constituents and nanoscale composite materials. In the latter case,

Fig. 5.7.10: Very-fine layered polymer blends.

the boundaries between classical materials classes will become obsolete and new properties will result from an ideal combination of several different materials, where the morphology and the hierarchical arrangement of the constituents will be the main parameter to tune properties. Nanotube-based systems are covered elsewhere in this document (see chapter 3.3.5), but many other systems are possible including nanoclay and graphite nanoplatelet systems. In many cases lessons will be learned from nature, where hierarchical structures have evolved and been used to good effect. Just recently, similar approaches have begun to be investigated (Fig. 5.7.12).

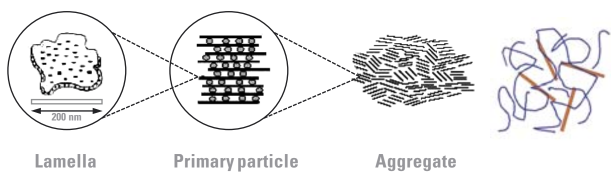

Fig. 5.7.11: Nylon nanocomposites can be made by exfoliating clays.

Critical needs for synchrotron radiation and neutrons

The production of nanostructured materials demands new manufacturing processes, or at the very least greater control over existing processes than we have at present. This must be based on sound science; science that can be established with the help of diffraction and scattering data providing kinetics as well as equilibrium thermodynamics. Critical to this is the ability to work under complex environments in real-time. More work needs to be done to make it easier for complex sample environments to be mounted on beam lines and for the data acquisition process to be synchronised with the experiment. This requires:

1. An opportunity for academics and industrial engineers to build in-situ rigs to study materials processing under synchrotron radiation and neutron supervision.
2. Nanotomography stations capable of viewing structural evolution in response to changes in processing conditions.
3. High intensity nano-microbeams to apply diffraction on nanostructures, fibres and coatings.
4. High spatial resolution SANS and SAXS techniques to map defect and precipitate variations across materials and components.

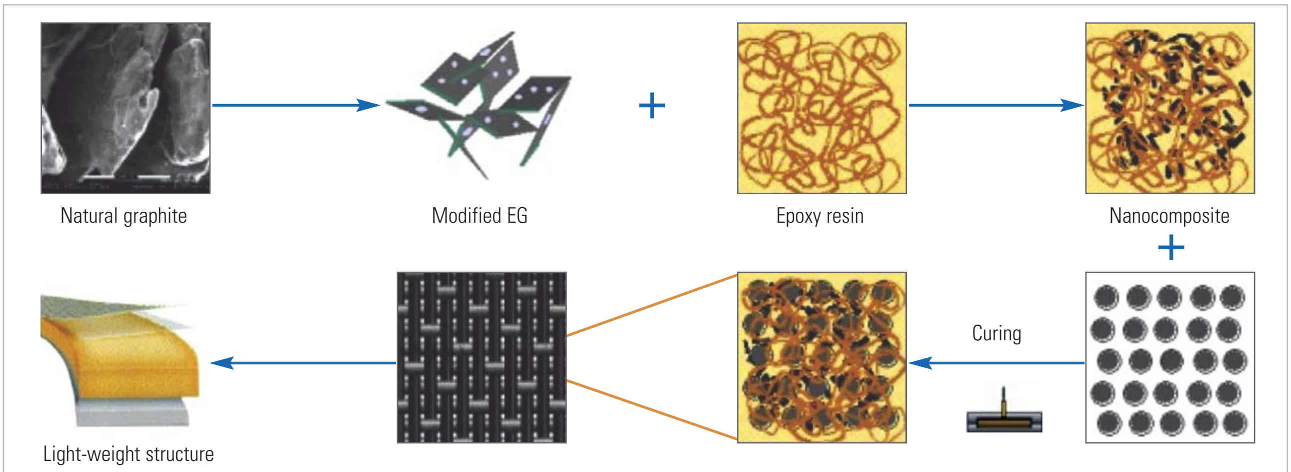

Fig. 5.7.12: Multi-scale structures.

- Intergranular strain development during forming
- Interphase strains in multiphase materials
- Identification of high-strain regions in forging
- Progress of internal reactions for in-situ structure formation

- Size distribution of nanoscale reinforcement
- Development of voids and damage on the nanoscale during processing
- Near-surface effects

In-situ diffraction measurements ↑ ↑ Small-angle, reflectometry and other methods

Neutron and synchrotron radiation techniques for the study of materials processing methods

In-situ and ↓ ex-situ tomography

Damage accumulation during processing · Phase distribution in multiphase systems · Density variation in powder processes · Monitoring of structure evolution

Fig. 5.7.13: Impact of neutron and synchrotron x-ray methods on process characterisation of composites and other multiphase structures.

5.8. TRANSPORT TECHNOLOGY: AIRCRAFT AND AUTOMOTIVE

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[Affiliations chapter 12]

Worldwide increase in the mobility of people and freight the demand for sustainable use of energy and mineral resources and the pressure to keep costs of transportation vehicles low, have lead to the development of transportation vehicles with a high level of functionality and sophistication. Materials for transport systems, exemplified here by automotive and aeronautic applications, have to meet a variety of demands regarding light-weight, stringent mechanical requirements, and temperature stability. Driven by stringent socio-economic pressure of future travel such as:

- Reduced fuel consumption, cost;
- Improved emission control, zero-CO_2;
- Increased capacity, mobility;
- Improved noise pollution, safety and passenger wellness/comfort;
- Protection of natural resources, environmental compatibility.

For civil aerospace applications, these requirements are embedded in the ACARE goals (See Fig. 5.8.1).

In many applications, e.g. aero-gas turbines, materials are now the limiting technology. Goals, such as those expressed in ACARE, can not be achieved without step-change advances in materials technology. This requires a novel approach to materials engineering, such as that offered through nanotechnology.

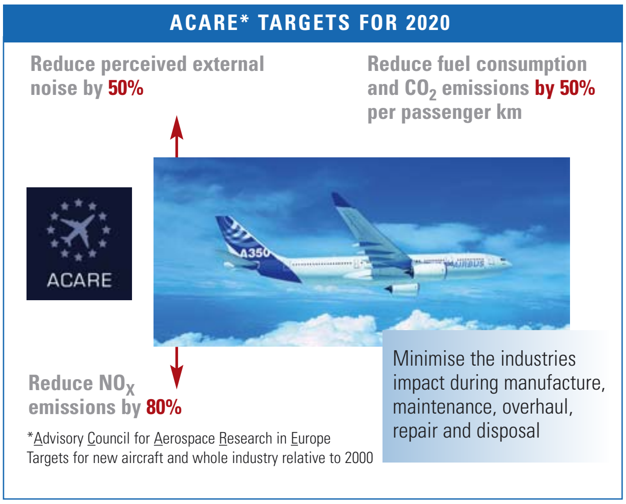


Fig. 5.8.1: Diagramme showing goals presented by the Advisory Council for Aerospace Research in Europe (ACARE).

The structural properties of materials are increasingly coupled with functional properties, which is the hallmark of nanotechnology, e.g. carbon nanotube, enabling and at the same time requiring often radical new design approaches to aircraft.

Nanotechnology has enormous potential to improve the reliability and performance of aerospace hardware while lowering manufacturing and service costs. Embedding nanoscale electromechanical system components into earth-orbiting satellites, planetary probes, and piloted, unmanned vehicles potentially could reduce the cost of future space programmes. The miniaturised sensing and robotic systems would enhance exploration capabilities at a significantly reduced cost, and most aerospace companies are actively investigating smart materials, molecular electronics, nanosensors, and other novel molecular devices exploring application concepts to improve the safety and efficiency of flight and quantifying the impact of, e.g., carbon nanotube reinforced polymers (CNRP), composite airframes.

For reasons of security and safety, the pressure on sophisticated materials is higher in the aerospace sector compared to automotive technology. Spin-off from the aerospace sector into other areas of technology is usual practice. A similar trend can be expected for nanotechnology, and this section will focus on the aerospace sector.

5.8.1. FUTURE TRENDS FOR NANOMATERIALS APPLICATIONS IN AERONAUTICS: AIRCRAFT, ENGINE AND AUTOMOTIVE

It is widely accepted that advances in computation, sensing, and aircraft materials are especially carried by innovations in nanotechnology (see Fig. 5.8.2).

Conventional materials will be improved or replaced by nanoscaled, nanostructured components or compounds; materials exclusively built out of nanoparticles, electronic devices using nanoscaled components will have significantly higher performance with an overall lower manufacturing cost.

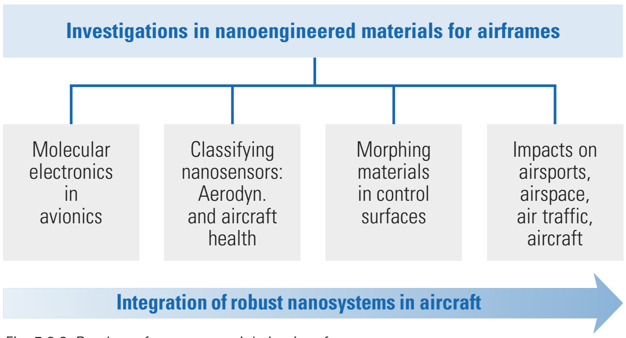


Fig. 5.8.2: Roadmap for nanomaterials in aircraft.

Potential applications of nanomaterials in aerospace and automotive include:

- Improved conventional and future design through new structural materials, wear resistant features, functional coatings;
- Supporting electronic devices;
- Advanced propulsion techniques;
- Carbon-nanotubes as actuators for adaptronics;
- Nanostructured thermoelectric functional materials (skutterudites, silicides);
- Nanoscaled thin films for gamma titanium aluminides;
- Mechanical alloying of light metal alloys with nanoparticles;
- Nanoparticles for conditioning of matrix systems of fibre-matrix-composites.

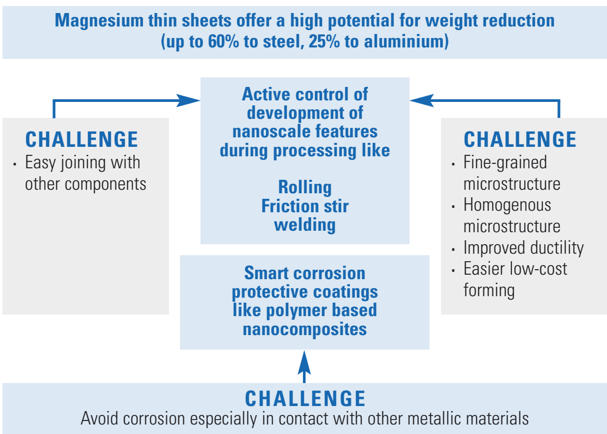
- Coatings and paints of various thicknesses;
- Hybrides and joints of different materials such as metal tubes containing ceramic foams;
- Bio-compatible interior;
- Embedded actuation: enhanced displacement, potential of morphing materials;
- Improve aerodynamic efficiency;
- Localised sensing – enables continuous airframe health monitoring
- Possibly increases airport productivity with lower aircraft maintenance time.

The importance of nanotechnology for the successful implementation of magnesium alloys for automotive and aerospace applications is demonstrated in the Fig. 5.8.3.

5.8.2. NANOMATERIALS IN AIRCRAFT AND SPACE STRUCTURES

This section gives in tabular and graphic forms:

- An overview of potential nano-materials: metallic-, ceramic-, polymeric- and coating materials in future aircraft (see Fig. 5.8.4);
- The research needs and the roadmaps for the next decade (see Fig. 5.8.5);
- A picture of a plane with an indication of the future nanomaterials usages (see Fig. 5.8.6).



Magnesium alloys for aerospace and automotive

Potential of magnesium alloys:

Mg offers the highest potential weight reduction in the entire field of transportation if three major limitations can be overcome:

- The presently insufficient high-temperature properties above 150°C must be substantially improved, potentially by inclusion of nanoscale particles;
- Difficulties in processing of thin Mg sheets have to be solved, potentially by nanoscale microstructure control;
- Vigorous corrosion (in combination with other materials) has to be controlled, e.g., through protective polymer-based nanocomposites and ceramic coatings.

Fig. 5.8.3: The importance of nanotechnology for the successful implementation of magnesium alloys for automotive and aerospace applications.

MATERIAL	NANOTECHNOLOGY	BENEFIT	TYPICAL MATERIALS
Metallic materials & Metal Matrix Composites	• Nanoalloys • Nanoceramics • Nanomultifunctional materials	• Improved strength/ toughness • Corrosion resistance • Temperature resistance	• Nanoparticle-, short fibre- & whisker reinforced Al, Ti & Mg matrix • Metal-ceramic nanostructured composites and coatings • Cellular metallic materials with gradient geometry • Nanostructured metals & Al-alloys via plastic deformation • Nanoporous metallic materials for multifunctional applications • $TiGaL_4V/TiB$ nanoenhanced composites • Nanoreinforced Mg alloys via powder metallurgy • NANOCERMET nanostructured bulk composites & coatings
Bulk metallic glasses & partially crystallised metals			• Rapidly solidified Zr- & Ti-based metallic glasses
Shape memory alloys			• NiTi intermetallics
Surfaces/coatings/sensors	• Nanolayers • Coatings containig nanoparticles	• Corrosion resistance • Shielding: electrical and optical • Defect signalisation: impacts, strain, dynamic loads • Functional coat (wear, dirt, bacteria, thermal protection)	• Paints with piezo-effective nanofillers, e.g., lead-zirconate-titanate

Fig. 5.8.4: Overview of nanomaterials in future aircraft.

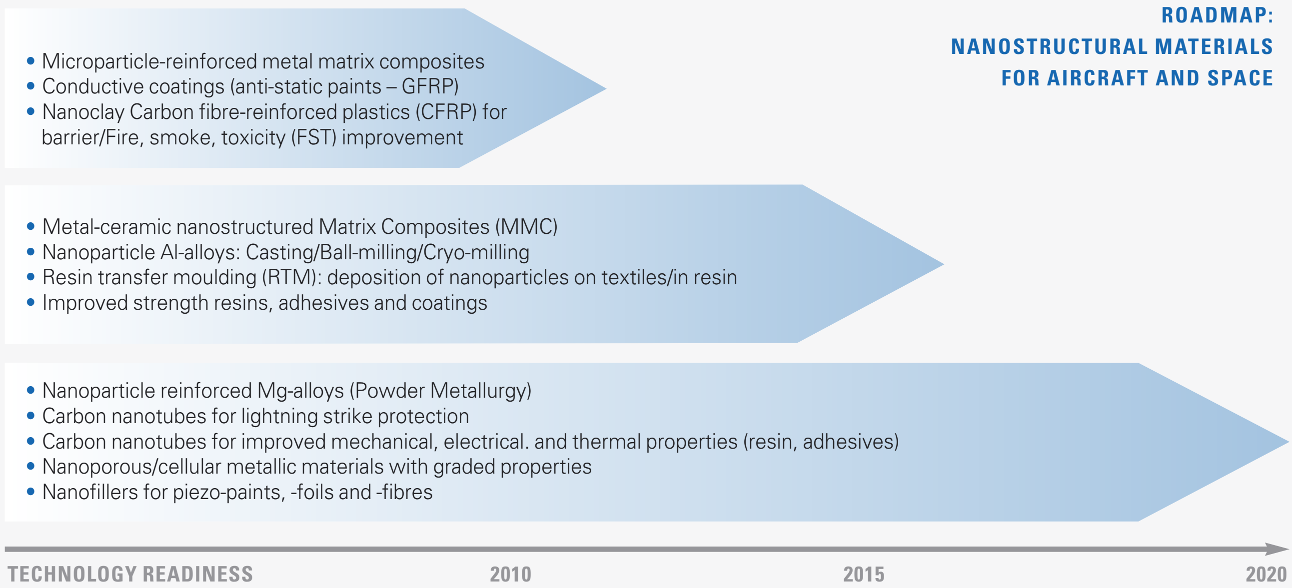


Fig. 5.8.5: Roadmap: Nanostructural materials for aircraft and aerospace technology.

Fig. 5.8.6: Nanomaterials applications in aircraft.

5.8.3. NANOMATERIALS FOR AEROENGINES

Aeroengines require increased engine performance and efficiency, with reduced environmental impact and through life cost. These translate to reduced fuel burn and emissions, through enhanced thermodynamic and propulsive efficiency, and cost-effective technologies to deliver long life components with minimum maintenance requirement (see Fig. 5.8.7).

From the viewpoint of materials technology, the requirement is always for increased strength and temperature capability, with reduced density and cost. Additionally, the duration of the development cycle for new materials must be reduced and the predictive capability and behavioural understanding enhanced.

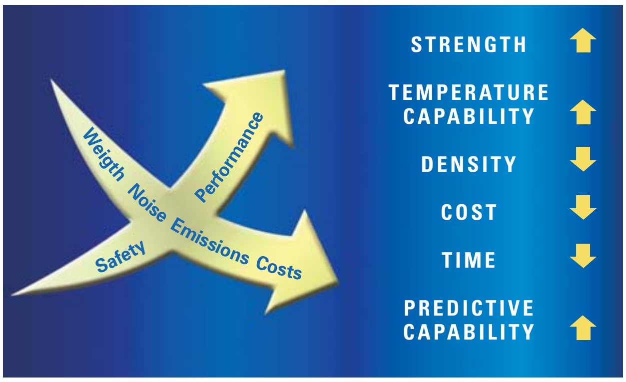


Fig. 5.8.7: The drivers for aeroengine technology.

Nanotechnology has the potential to deliver a step change in capability against a number of the above goals through the opportunity to take a systems design approach, tailoring the structure and properties of a component to its operating environment.

The main potential applications for nanotechnology with the aero-engine are summarised in Fig. 5.8.8:
- Nanodispersion strengthened alloys;
- Nanostructured protective coatings;
- Multi-functional materials for adaptronic designs;

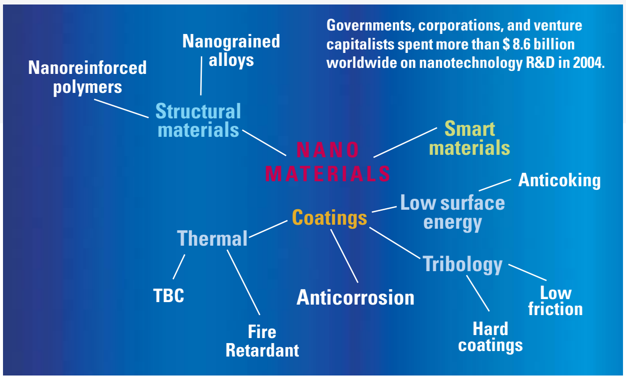


Fig. 5.8.8: Manipulating atoms to make materials.

- Designed Microstructures: nano-processing, modelling, testing;
- High temperature nanofunctional materials for sensors and actuators;

Within the broad field of nanotechnology, nanostructured coatings perhaps offer the greatest potential (see Fig. 5.8.9 and Fig. 5.8.10).

- **Thermal barrier coatings (TBC) and corrosion protection**

See Fig. 5.8.11. Control of coating structure at the nanoscale offers a route to deliver coatings, for combustor and turbine components, with controlled thermal conductivity, enhanced component life and for marine and industrial applications, in particular enhanced corrosion resistance. Component life can be extended through coatings resistant to sintering and engine-related degradation, i.e., erosion, FOD and CMAS. This could be achieved through the design of structures that suppress heat transfer paths and/or have modified surface chemistry and energy absorbing capabilities within their structure.

- **Tribological coatings**

Coatings could deliver advanced wear resistance both in metal to metal interactions and under conditions of erosive wear, i.e., compressor aerofoils. Potential routes would include low friction coatings, hard coatings and multilayer coatings, engineered to deliver energy absorption without a fatigue debit.

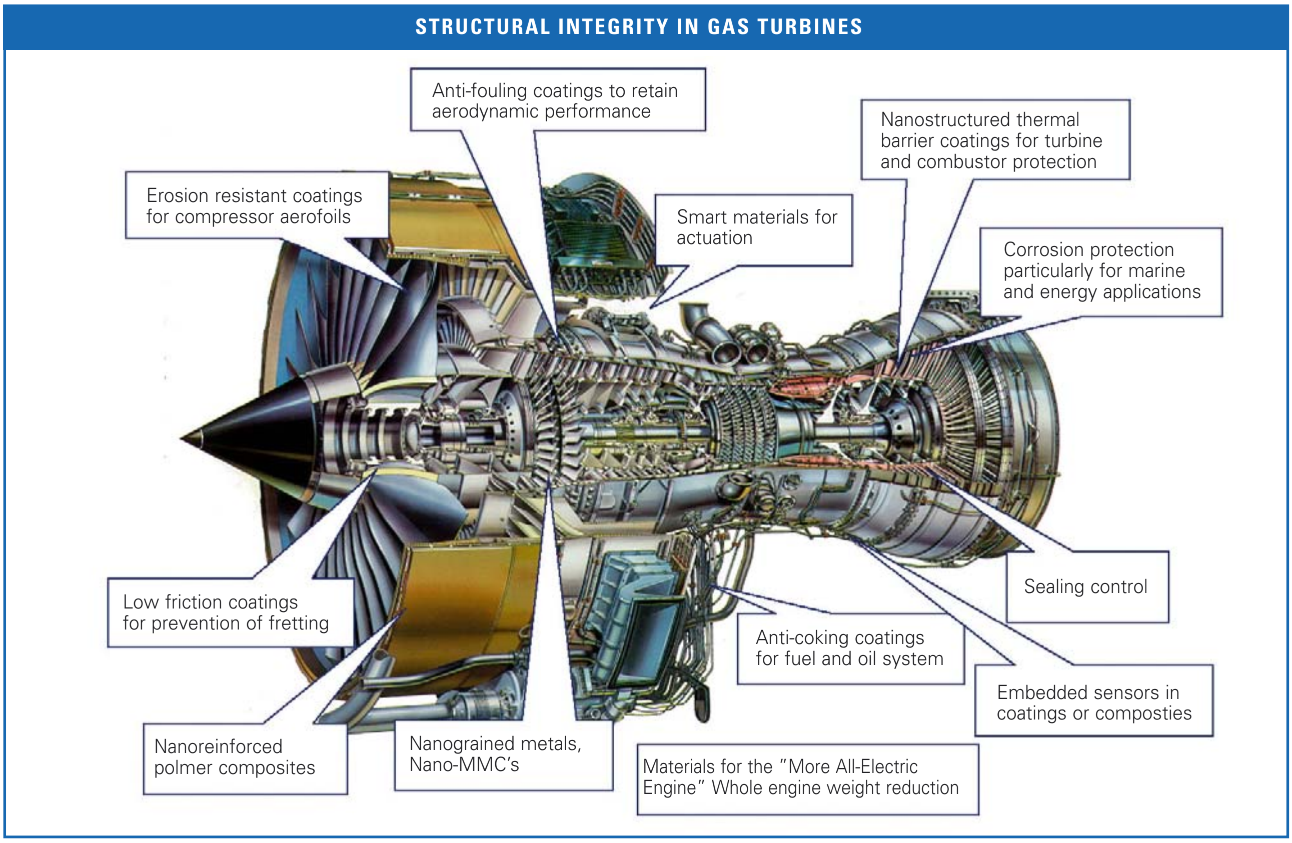


Fig. 5.8.9: The role of nanomaterials in the aeronautics propulsion systems sector.

COATING TYPE	APPLICATION	BENEFIT	TARGET
Adv. TBC	Combustor/HP turbine	Enhanced efficiency, reduced fuel burn, emissions and op. costs	-50% thermal conductivity x10 life increase vs engine degradation
Corrosion resistant	HP/IP turbine	Reduced op. costs, enhanced reliability.	x5 life enhancement
Wear resistant	Blade fixings/transmissions	Reduced op. costs, enhanced reliability.	No recoat/refurb. required for full engine life
Erosion resistant	Compressor aerofoils	Reduced op. costs, enhanced reliability.	x10 life enhancement
Anti-fouling	Compressor/fluid systems	Reduced op. costs, enhanced efficiency, and enhanced reliability.	Eliminate requirement for maintenance intervention i.e. comp. wash

Fig. 5.8.10: Applications summary for nanostructured coatings.

Coatings for high-temperature protection in aerospace

Oxidation protective layers and thermal barrier coatings allow substantially increased operating temperatures and hence energy efficiency in aeroengines, power trains and stationary gas turbines. To allow the optimised design-in of these layers the following limitations have to be overcome:

- Uncontrolled failure of high-temperature oxidation protective layers must become predictable and time-to-failure has to be prolonged substantially. Most promising technology is the application of nanolayers of protective oxides.
- Almost stochastic failure of thermal barrier coatings has to be replaced by long-term reliable design. Most promising technology is based on nanostructuring of internal inter-phases and stress-control in the nanometre range.

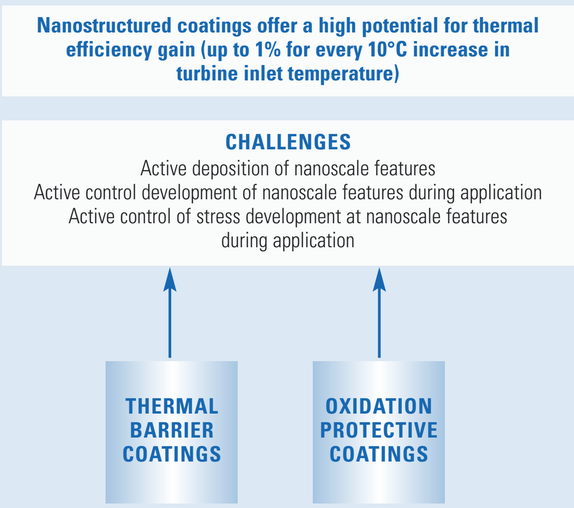


Fig. 5.8.11: The importance of nanotechnology for the successful implementation of high-temperature coating alloys for aerospace applications.

- **Smart coatings**

Coatings could be envisaged with embedded sensor capability for stress, temperature, pressure, air flow, etc. These could enable in-situ data gathering and transfer while the engine is in service.

The growth of nanostructures to enhance turbine and compressor sealing may be possible, with the potential to incorporate active clearance control and with a benign impact on downstream engine components, i.e., from wear debris.

Research needs

Critical to all of the above is the ability to interrogate nanoscale materials to understand and optimise manufacturing/structure/property relationships via a "nanomaterials database".

This will require an advanced tool set to enable the characterisation of nanoscale structure, defects and stress state and the response to mechanical loading and environmental factors. The ability to examine materials at extreme resolutions under dynamic loading and under representative temperatures/environments will be critical.

Further downstream technology validation will require the capability for component testing under simulated engine conditions and the examination of rig/engine-run demonstrator components.

Throughout the development and validation cycle, the capability for materials modelling to shorten development cycles, enabling early introduction to service, and underpinning behavioural understanding and hence component integrity is key.

5.8.4. NANOMATERIALS IN AUTOMOTIVE TECHNOLOGY

The need for nanomaterials in automotive technology is summarised in the following diagrammes (see Figs. 5.8.12 and 5.8.13).

5.8.5. CONCLUSIONS

- To allow successful research on future breakthrough of nanomaterials, advanced neutron and synchrotron x-ray characterisation techniques are required. This promises to improve future transportation systems by implementation of, e.g., functional light-weight materials, new propulsion concepts, integrated avionics and devices resulting in significant weight reductions in aeronautics and transport creating major savings in energy and CO_2 emission in the near future. They will contribute to economic viability and sustainable development.

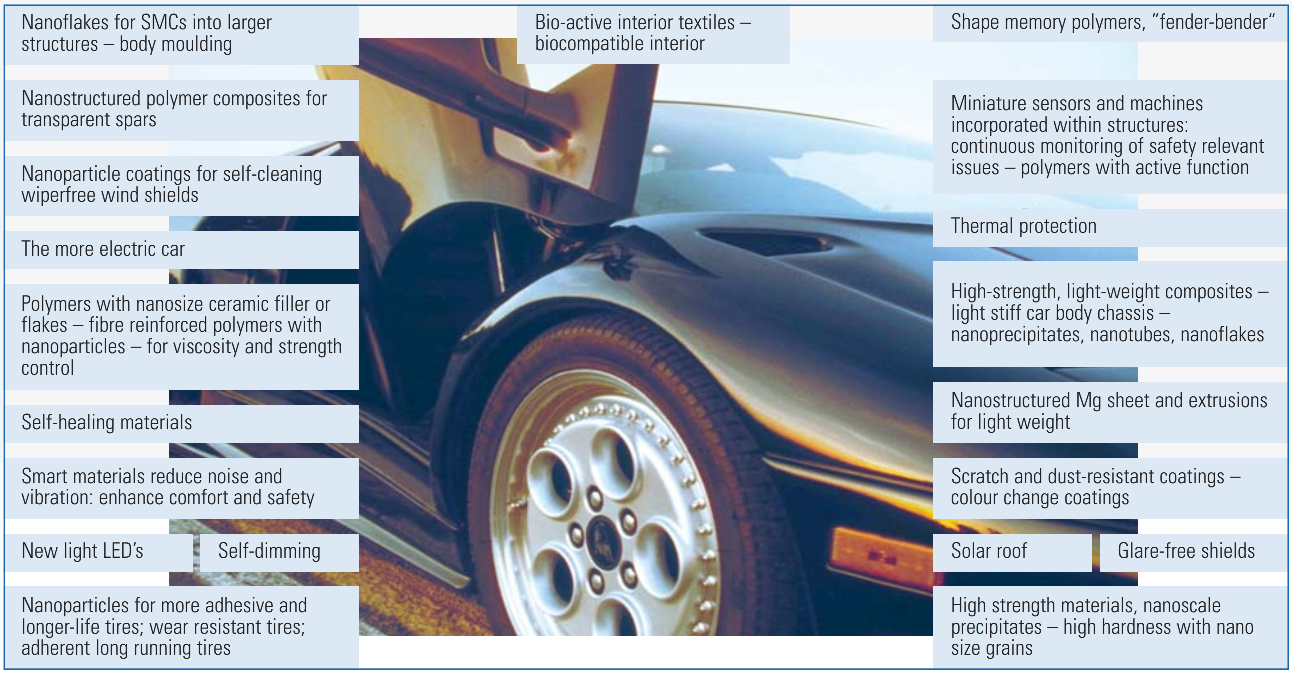


Fig. 5.8.12: The role of nanomaterials in the car structure.

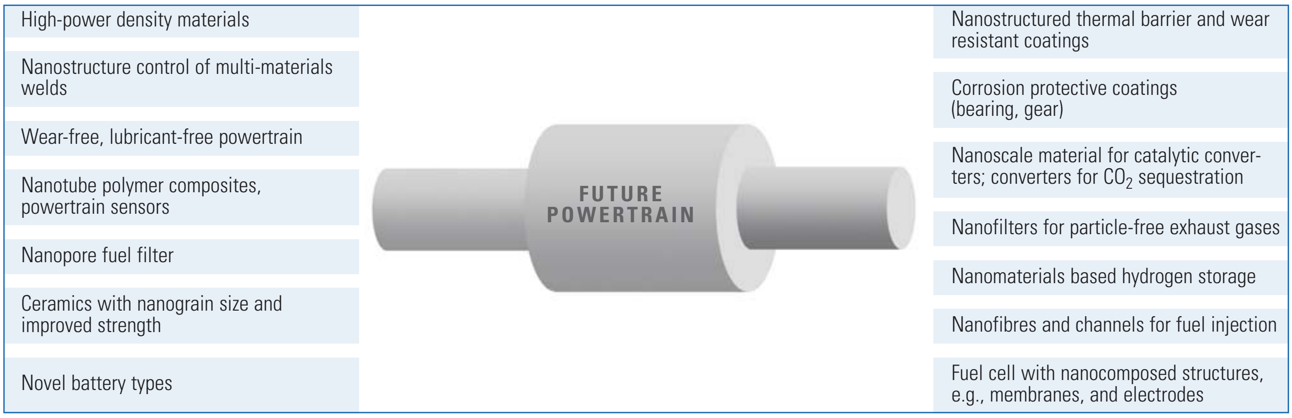


Fig. 5.8.13: The role of nanomaterials in the automotive engine.

- The creation of new research synergies and a closely correlated efforts of both the materials science community and the large-scale facilities in the use of synchrotron and neutron methods will pave the way to major breakthroughs in nanomaterials science and technology. This is of vital importance for the future competitiveness of Europe in the area of transportation vehicles. This can be partly realised by the creation of centres of excellence at selected research facilities.

Creation of a technology platform for "advanced coatings"

The development of advanced coatings is a key for design of high-tech components for automotive and aerospace technologies. For making a substantial progress in the design of new coatings, new concerted efforts between the automotive and aerospace industry, the key research laboratories for thin film science and the synchrotron radiation and neutron facilities have to be made. The enormous challenges in this enterprise are best met by the creation of a technology platform at a large scale facility led by an industrial consortium which integrates:

- All necessary technologies to design new coatings and to characterise their structure – function relationship;
- A facility for systematic testing of the performance, lifetime and failure mechanisms of coatings;
- A combinatorial coating design capability.

This platform should strongly interact with the Science Centres for "Functional Interfaces" and "Precision Synthesis".

CHALLENGE	BREAKTHROUGH	KEY BARRIER
Non-toxic corrosion resistant surface paint for aircraft fuselage	Self-assembling silanes or similar materials and composites for multi-layer functional coatings	Synchrotron radiation and neutrons equate to self-assembling timescales
"Design-in" thermal barrier coatings for rotating turbine blades with predictable failure behaviour	Design coating components on the basis of known defect and stress development in thermally grown oxide layer	Synchrotron radiation tomography of defects in thermally grown oxide layer and stress analysis on a scale of less than 100 nm
Successors to heavy Ni-super alloys in aeroengines with increased temp. capability; High performance, light-weight metals and composites for lower temp. application, e.g., aeroengine compressor	Controlled design of microstructure and processing on the nanoscale level	Synchrotron radiation and neutron probes for texture and strain measurements with high spatial (<100 nm) resolution.
Materials for more electric aeroengine technology	Design of nanostructured high-strength alloys with superior thermal conductivity	Synchrotron radiation and neutron probes for texture and strain measurements with highspatial (<100 nm) resolution

Fig. 5.8.14: Challenges in the aeronautics sector and the contribution from synchrotron radiation and neutrons.

The need for neutron and synchrotron x-ray radiation to study aerospace and automotive nanomaterials and components

Progress in nanomaterials science and technology demands for synchrotron radiation and neutron sources. The most prominent challenges for a progressive use of neutrons and synchrotron x-rays as characterisation probes for nanomaterials in the field of basic research for space and automotive as well as in the field of component reliability and routine industrial use – in particular in harsh environments – are outlined (see Figs. 5.8.14 and 5.8.15):

- Determination of diffusion mechanisms by means of determination of activation energy and diffusion coefficient, e.g. in partially-stabilised zirconia (PYSZ) material for thermal barrier coatings (TBC);
- Analysis of thermally induced changes of the nanostructure in thermal barrier coatings;
- High temperature investigation for in-situ phase analysis of TBC bond coat degeneration;
- Interface sensitivity to characterise coatings: different layers;
- High-resolution stress and texture measurements: with spatial resolution matching grain size;
- Time-resolved high temperature experiments/environments for in-situ analysis of the kinetics of phase transitions of nanostructured iron di-silicide ;
- Exploring lattice disorder with neighbouring mass number elements (phase/element contrasting);
- Sub-ångstrom resolution to detect atomic positions and strains
- High-resolution tomography of larger ceramic matrix composite components;
- Analysis of intrinsic stresses in light metal alloys by diffraction;
- Real-time observation: formation of nanopores, distribution of nanoparticles/nanopores in complex geometries;
- Experiments in industrial simulating environments;
- Ultrafast data acquisition to investigate, e.g., casting or welding processes in real-time;
- High local resolution to detect inhomogeneities and gradients;
- Study of thermoelectric materials for high temperature thermal sensors and auxiliary current sources (thermoelectric energy conversion);
- In-situ analysis of mechanism of incorporation and transports of nitric oxides in multiple nanolayers for NO_X gas sensors and catalysts;
- Penetration power, to investigate parts and components of all desirable sizes in a non-destructive way;
- Standardised and certified procedures and measurements;
- Simultaneous use or combination of diffraction/tomography/small angle scattering;
- Development of faster and more efficient detector systems.

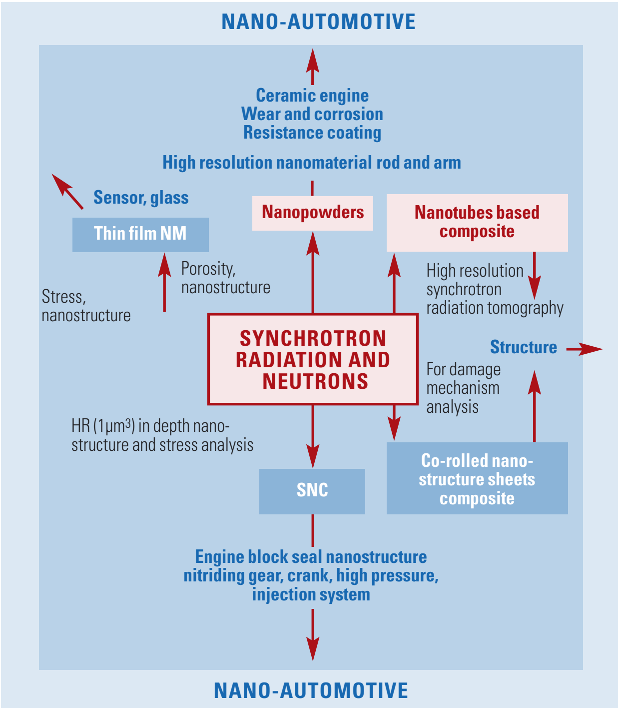


Fig. 5.8.15: Challenges in the automotive sector and the contribution from synchrotron radiation and neutrons.

5.9. ENVIRONMENT

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5.9.1. NATURAL ENVIRONMENT

Maintaining and restoring the quality of water, air and soil, so that the earth will be able to sustainably support human and other life, is one of the great challenges of our time. The scarcity of water, both in terms of quantity as well as quality, poses a significant threat to the well-being of people, especially in developing countries. Environmental nanotechnology is considered to play a key role in the shaping of current environmental engineering and science. Looking at materials at the nanoscale has stimulated the development and use of novel and cost-effective technologies for remediation, pollution detection, catalysis and others. There is the huge hope that nanotechnological applications and products will lead to a cleaner and healthier environment. Great hope is also placed on the role that nanotechnology can play in providing efficient and cheap access to clean water for developing countries.

Particles in the nanosized range have been present on earth for millions of years and have been used by mankind for thousands of years. Fig. 5.9.1 shows that nanoparticles occur naturally in the environment in the atmosphere in the form of aerosols, in aquatic systems as colloids, and in soils and the subsurface in a variety of biogenic and geogenic materials. Nanoparticles are also formed as an unintended by-product from human activities during combustion of fossil fuels or biomass. All these types of nanoparticles are also deliberately produced as engineered nanoparticles, in addition to a wide array of newly synthesised forms. These particles are either released unintentionally into the environment or are introduced on purpose, e.g. during remediation of polluted soils.

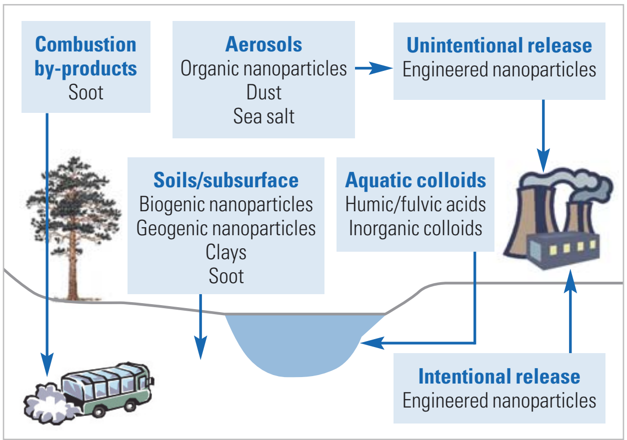

Fig. 5.9.1: Occurrence and sources of nanoparticles in the environment from natural and anthropogenic sources.

Future trends in nanomaterials research and technology

Nanoparticles are both a hope for new processes in environmental engineering and the topic of anxiety regarding the threat or risk they may pose to the environment. Both are linked to the specific properties of their surface which differ from that of larger particles. In order to predict surface nanoparticle properties, one needs to understand their organisation and properties at different scales. The key challenges are:

Exposure, environmental fate and transport

Nanotechnology exposure, environmental fate, and transport will be fundamental in determining overall environmental impact. The transport of nanoparticles will depend, as with single ions or molecules, on their interaction with mineral, organic or biological surfaces.

Thermodynamic and stability aspects of nanomaterials

The solubility of nanoparticles differs from that of larger particles due to surface tension effects. In particular surface derivatizations have the potential to greatly alter the solubility, toxicity and catalytic properties of underlying nanoparticles. Understanding ageing, dynamic processes of physical change (such as aggregation, structural transformation and crystallisation or "ripening"), phase separation and chemical reactions that occur on a wide range of timescales, is becoming more and more important and requires systematic in-situ and long-term studies exploiting the non-destructive capabilities of modern synchrotron radiation and neutron techniques.

Toxicity risk linked to nanoparticles

The interaction between nanoparticles and the human body is currently poorly understood. System biologists are beginning to understand better what takes place during the interaction of cell membranes and cell organelles with nanoparticles using scientific concepts such as genomics, proteomics, and metabolomics. The convergence of these biological sciences with nanotechnology offers opportunities to fine-tune the toxicological risk. The toxicology of nanoparticles is often linked to the production of free radicals. There is the need to couple such toxicity tests with studies on the aggregation of nanoparticles. Thus, studies aiming at correlating the micro- and nanostructure with its toxicological properties, including the interpretation of properties in terms of structure and interactions of nanoparticles in various biological mixed systems, make a strong case for to continuing with the toxicity assessment of these particles.

Environmental nanotechnology

Environmental systems such as soils or sediments are often complex composite materials involving organic and mineral structures, which constitute important barriers towards pollutions. In order to exploit and enhance these natural strategies with nanoparticles and nanotechnology in environmental nanotechnology, we need more structural information, which can ideally be provided by synchrotron radiation and neutron facilities, if the appropriate analytical environment is delivered.
Potential breakthroughs include understanding/developing the following:

- Structure of water and ions at the surface of nanoparticles;
- Structure of components present within nanomaterials;
- Molecular adsorbents in practical applications to control crystallisation;
- Long-term gel stability as a function of time and temperature fluctuations;
- Developing diffusion concepts for the use of nanoparticles as targeted pesticide delivery systems;

- Nanoencapsulation systems (adopted from the pharmaceutical industry) to protect, mask and/or deliver specific nutrients to plants and micro-organisms where they have maximum effect;
- Special indicators utilising nanotechnology to colorimetrically signal redox status in various environment;
- Sieving of 1-D crystal (in the same way zeolites were used in the catalytic industry to sieve specific organic molecules);
- Control of the cross-linking of protein and/or polysaccharide fibrils in nanoparticles and the emergence of life.

Soil and groundwater remediation

The use of nanoscale zero-valent iron (nZVI) for groundwater remediation represents the most investigated environmental nanotechnological technique. Granular zero-valent iron in the form of reactive barriers has been used for many years now at numerous sites all over the world for remediation of organic and inorganic contaminants in groundwater. Other nanoparticles are proposed for the remediation of soil polluted with organic and inorganic contaminants.

Water treatment

Clean water is a requirement for all properly functioning societies worldwide, but is often limited. New approaches are continually being examined to supplement traditional water treatment methods. These need to be lower in costs and more effective than current techniques for removal of contaminants from water. In this context, nanotechnological approaches are also considered. Nanoparticles are used as potent adsorbents, in some cases combined with magnetic particles to ease particle separation; nanoparticles used as catalysts for chemical or photochemical destruction of contaminants; nanosized zero-valent iron used for removal of metals and organic compounds from water; and nanofiltration membranes. The most effective methods are likely to consist of more than one of these technologies in a hybrid system.

Air purification

Indoor as well as outdoor air pollutants must be considered. Photocatalysis reactions at close to ambient temperature can be used to degrade air pollutants. Incorporation of photocatalytic nanomaterials in building materials or paints gives them self-cleaning and de-polluting properties. When exposed to solar radiation they act as catalysts for photodecomposition of pollutant molecules into non-toxic compounds. The most important areas of research are self-cleaning paints and glasses, anti-fogging coatings, antibacterial effects, and air purification applications. A better knowledge of the mechanisms of photodegradation and photocatalytic efficiency of the materials is needed, together with testing both at the laboratory scale and under everyday-life conditions.

Pollution detection and sensing

Various nanostructured materials have been explored for their use in sensors for the detection of different compounds. These sensors will be used for cheap and on-line detection and control of pollutants in water and air. The merging of nano- and biotechnological systems, together with advanced information technology, will be especially promising.

More efficient resource and energy consumption

Pollution prevention by nanotechnology refers on the one hand to the reduction in the use of raw materials, water or other resources and the elimination or reduction of waste, and on the other hand to more efficient use of energy or improvements in energy production and storage. The implementation of green chemistry principles for the production of nanoparticles and for nanotechnological applications in standard chemical engineering will lead to a great reduction in waste generation, less hazardous chemical syntheses, improved catalysis and finally an inherently safer chemistry.

Nanomaterials can be substituted for conventional materials that require more raw materials, are more energy-intensive to produce, are less abundant, or are known to be environmentally harmful. Some new nanocatalysts can be used at much lower temperatures than conventional catalysts and therefore require less energy input. The capacity of nanocatalysts to function at room temperature opens the way for broad applications of nanomaterials in many consumer products. Nanotechnology may also transform energy production and storage by providing less environmentally damaging alternatives to current practices.

Research roadmap

The following aspects related to using nanomaterials for the environment will need to be addressed at the same time, allowing the results of one area to influence the development of the other field:

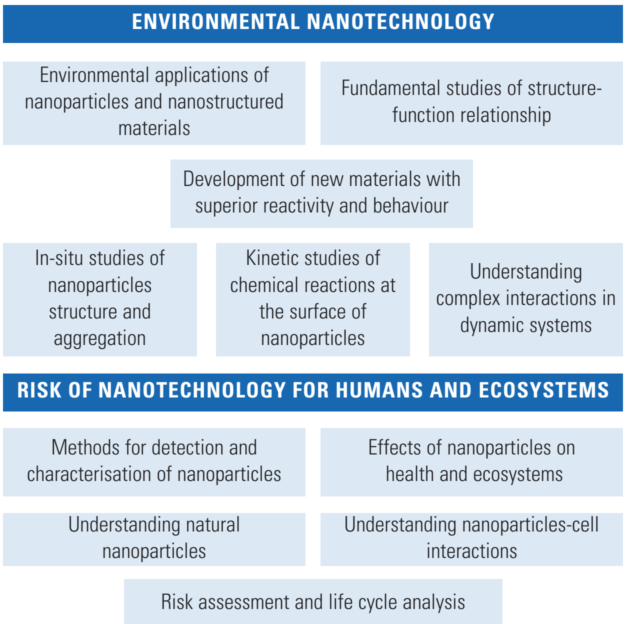

Fig. 5.9.2: Research roadmap for applications of nanotechnology in the environment and the risk of nanotechnology for humans and ecosystems.

General conclusions and recommendations

Because environmental research is a multidisciplinary field, a single effort or centre cannot address all the key challenges. It is at the nanolevel that physical changes and interactions with contaminants determine the designed decontamination process efficiency. Therefore, an integrated and multidisciplinary approach of key problems in environmental research and industry is required.

In order to make progress, partnerships between environmental industry and nanoscientists are mandatory. Moreover, at least a European Environmental Network is needed or, even better, a European Institute for Environmental Science, distinct from the Copenhagen European Environmental Protection Agency, dedicated to monitoring and policy.

The environment can only be studied successfully when research is to be extended from structural and compositional studies to studies of environmental dynamics. This work will involve time-resolved structural studies by means of small-angle scattering, diffraction, imaging and tomography. Mostly, parallel use of different techniques and the application of complicated external conditions based on concentration and hydraulic potential gradients will be necessary.

These conclusions should at least materialise in:

- Instrument development at large-scale facilities for multi-technique analysis, in real-time, under conditions simulating appropriate engineering strategies, dedicated to decontamination problems and waste management;
- A network of interdisciplinary researchers involved in the study of the interplay between micro- and nanostructure made of nanoparticles and NT, cells and upper organisms;
- Enhanced cooperation between environmental experts from the waste and water industry, academia, and the scientists at the large-scale facilities;
- High priority on environmental research, also in the allocation of beam line access at research facilities.

Nanotechnology will help solve some of the pressing problems of this century in a rapidly changing world needing to adapt to a sustainable way of living. Environmental nanotechnology can particularly help in the following applications fields:

- Supply of clean water for the world in a cheap and efficient matter;
- Treatment of groundwater and waste water;
- Indoor and outdoor air purification by photocatalysis;
- Cleaning and restoration of affected and polluted natural resources (water, air, soil);
- Monitoring the state of the environment through cheap real-time pollutant analysis using low-cost sensors and biosensors;
- Prevention of pollution through cleaner, less wasteful manufacturing and the use of less toxic materials;
- More efficient catalysts to help reduce industrial and vehicle emissions;
- Cleaner and more efficient energy production and storage systems;
- Methods of CO_2 sequestration by reaction with nanostructured minerals.

Role of synchrotron radiation and neutrons

Synchrotron, x-ray, and IR- radiation is increasingly used to characterise complex environmental materials, in particular when those materials are in unusually extreme environments (reactive medium, biological growth medium, high pressure and salinity). Nanoscience asks for a fundamental understanding of the interaction between particles and liquids (or gases) at the various length scales. This task requires the development/use of advanced analytical technologies (Table 5.9.1).

With increasingly tighter regulations, environmental sustainability will demand clever design. As the future challenges lie in the nanometre regime, it is imperative that environmental science and technology should have the appropriate analytical tools available to explore the nanostructure of contaminant and engineered decontamination processes.

LEVEL	LENGTH SCALE	ENVIRONMENT LEVEL	SCIENTIFIC FIELDS	ANALYTICAL TOOLS
Atomic	Ångstrom		Analytical chemistry Structural chemistry Crystallography	EXAFS, XANES NMR, XRD AFM
Molecular	0.1–1 nm	Single NP and NT	Analytical chemistry Structural chemistry	EXAFS, XANES NMR, XRD, WAXS Mass spectroscopy
Macromolecules	1–100 nm	NP aggregates and interaction with, e.g., cell materials	Physical chemistry, Molecular toxicology	Light scattering SANS, SAXS, WAXS Electron microscopy
NP assemblies, e.g., with filters of cells	0.1–10 µm	Water and waste treatment; interaction with plants, or lungs	Physical chemistry Process engineering Toxicity tests	SANS, SAXS Optical and electron microscopy

Table 5.9.1: Relevant length scales and complexity of nanoparticle products and their implication in the environment.

While electron microscopy related observations often involve highly specific sample treatments prior to "post mortem" structure visualisation and the risk for radiation damage, more recently developed experimental tools, such as synchrotron radiation and neutrons in combination with advanced microscopy tools (STM/AFM), will revolutionise the future progress in environmental sciences. Highly promising developments are in:

- X-ray and neutron reflectivity for probing surfaces and interfaces;
- X-ray microtomography to achieve a 3-D map of the porosity in natural and engineered materials;
- Elemental and redox mapping at the micron scale (μ-XRF, μEXAFS and μ-XANES) will allow visualising the complexity of any (atmospheric, soil, plant, microbial mat or sediment) particle system and their interactions with nanoparticles;
- Contrast variation, either by isotopic substitution in neutron diffusion experiments to probe the local environment, particularly the local water structure around a given atom, or by energy scattering to map the presence of a given element;
- Small angle neutron scattering to see within large structures fluctuations of density at the μm size level;
- 3-axis quasi-elastic scattering to follow fluctuation of density in water layers, e.g., in CNT;
- Neutron and spin-echo time of flying, to look at diffusion at the picoseconds or nanosecond, of, e.g., an organic molecule along a C surface (graphite or CNT).

Apart from the high potential to visualise structures with nanometre dimensions, there is the unique potential of synchrotron radiation and neutron technique to observe:

- Structural changes in real-time (typically down to milliseconds), under environmental-like "stopped-flow" conditions (water, flow, pressure, temperature) and in a destruction-free mode;
- Redox change in the same conditions, e.g. during oxidation of organic molecules.

Necessary developments

Areas that need to be addressed to maximise the potential of synchrotron radiation and neutrons in environment-oriented nanoparticle studies:

- Future achievements will depend strongly on the development of new tools capable of performing real-time simultaneous measurements at the nanoscale under realistic conditions. Effective communication between synchrotron radiation and neutron scientists and industry may lead to new analytical concepts.
- Current software is not able to cope with the vast amounts of data which result from time-resolved experiments and even from static measurements. Moreover, it would be a great advantage for on-the-run optimisation of time-resolved experiments if software were available that enabled real-time interpretation.
- Staff at facilities will need encouragement to interact and train new users from environmental nanoparticles science who will often come from backgrounds that are not related to synchrotron radiation and neutrons at all.
- Increased flux at neutron sources coupled with advances in optics development and counting devices could facilitate specific time experiments (involving contrast variation) under conditions realistically mimicking processing.
- The development of appropriate in-situ cells should reproduce environment-like conditions.
- Improved resolution of x-ray tomography and imaging in the "water window" will offer new opportunities for revealing high resolution x-ray images of the complex heterogeneous structure that makes up most environmental materials.
- Resonant x-ray imaging may help to reveal the location of minerals and trace elements after reaction, to help understand encapsulation and nutrient availability.
- Converging and multi-technique approaches must further be developed.

5.9.2. MAN-MADE ENVIRONMENT

Nanosciences challenges and role of technology for a sustainable development

Sustainable growth experienced in developed countries can not be generalised worldwide without dramatic consequences for future generations. One of the dramatic consequences of non-sustainable developments is the "climate change paradigm". Although many experts alert society about the potential consequences of climate change, both on humans, the economy, biodiversity and geopolitics, only few actions have been taken into account to fight against it. Within the possible strategies to fight against climate change, nanotechnologies can and must play a key role for:

1. **A better understanding of the role of nanoparticles in the mechanism of earth warming** (see section 5.9.4):
   - To better predict the relationship between climate, air quality and health;
   - To provide information about possible feedbacks within the earth system, that could take place in the near future or that can be used to counter-act climate warming (In 2006, NASA organised a high level conference with scientists involved in the climate change fight to expose their solutions, some of them were to counter-act the stratosphere itself, playing with the climate).
2. **A better use of natural resources,** as a first step in the overall system,
3. **A better re-use of intermediate waste in a worldwide "technological ecosystem"** in which the output of a technology/production/system chain can be seen as the input of another technological chain. CO_2 is a good example of what should be done: CO_2 is the major "society waste" regarding climate change, the chemistry of CO_2 should be addressed urgently through (see Fig. 5.9.3.) :
   - **CO_2 capture**: no system already exists to capture CO_2 in such condition that CO_2 can be re-used as an input for some chemical processes. Local as well as large-scale carbon capture are major challenges for tomorrow;
   - **CO_2 recycling and CO_2 -based process** can be developed at different stages using different physical, chemical and biological

principles. By way of example, algae or bacteria that can reduce CO_2 and hydrogen. CO_2-based processes can be used in many production systems (cement, alloys etc.). This "**carbo-chemistry**" will take place in the complete carbon chain after petrochemistry and aims for extracting carbon from natural resources;
- **CO_2 sequestration** is at the end of the chain, it is the extreme solution when the other solutions have failed.

Industrial ecology concept

The industrial ecology (IE) concept is basically a bio-inspired approach in which all along the food-chain a waste is used as a food for another species: All intermediate waste that is generated along the technological pathways should be used as the input of another technology. IE is an interdisciplinary field that uses system approaches to focus upon the relationship of industrialism to organisms and their environ-

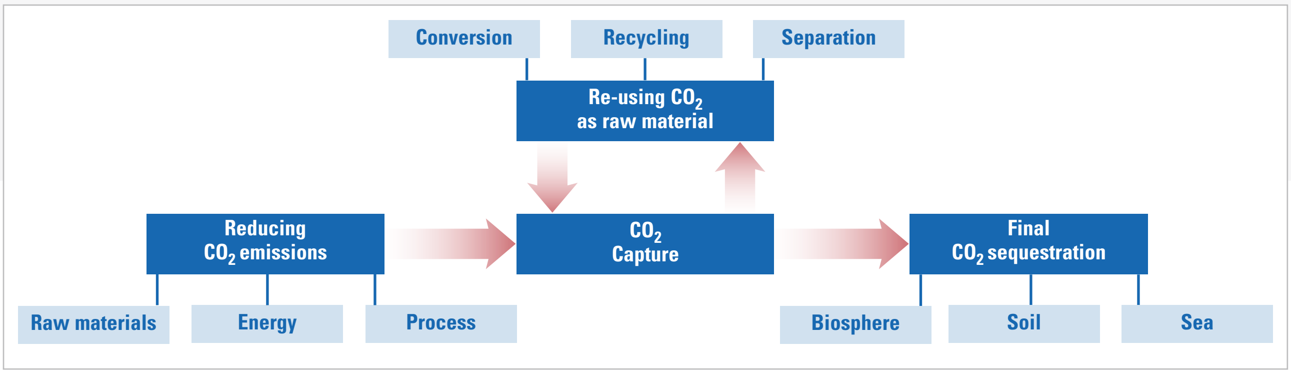

Fig. 5.9.3: The man-made Carbon cycle.

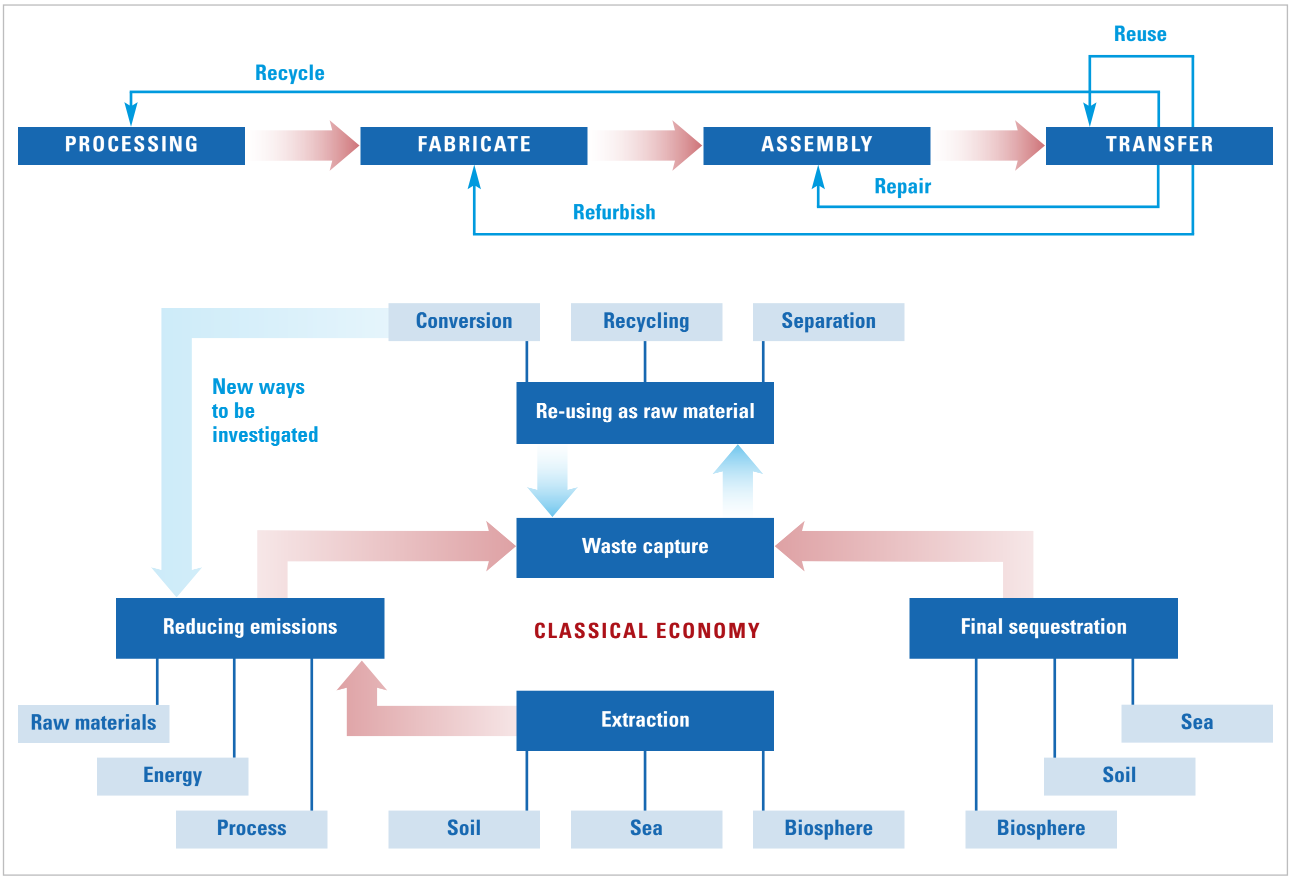

Fig. 5.9.4: Recycling roadmap

ment. IE promotes changes from a wasteful economy to a closed looped system of production and consumption. Through this mechanism, industrial, governmental and consumer waste is re-used, recycled, and remanufactured to the limits of knowledge and technology.

Nanotechnology can be used to manufacture inert and bio-objects. Similar to nature, bio-engineered "software" instructions will be the blueprint for the assembly and operation of products at the atomic level. The development of this technology carries the potential to disassemble existing and future waste (inert and bio-) to the molecular level, and then re-assemble it into new resources and products. This cyclical approach, if designed into the system, would show the raw materials used in objects to never reach end-of-life.

Fundamental research is mandatory to open new ways of conversion for all waste (gas, liquids, solids) so that energy or raw material can be kept at low costs. A current example is shown in Fig. 5.9.5.

In this concept, nanomaterial technologies and manipulation of matter at the nanoscale should play a major role, in particular for handling the urgent CO_2 problem: Nanomaterials and future nanotechnologies should be developed for:

- **CO_2 emission reduction**: Already well developed in many places
- **CO_2 capture**: Nanoscience is not well developed in this field of activity and an effort should be done to organise transdisciplinary conferences or exchanges between the geology community and the nanoscience communities. CO_2 capture has been done mainly through a large-scale approach, trying to capture CO_2 directly in the atmosphere. A more decentralised and local approach can be emphasised. Few initiatives have been launched to capture CO_2 directly at the output of plan chimneys, this can be generalised for instance at every car motor a number of nanomaterials (see Fig. 5.9.6) can be good candidates such as:
  - Solvents/sorbents: both physical and chemical which could help design several solutions for CO_2 reduction or storage i.e. ionic liquids, role of liquid interfaces etc.;
  - Robustness with respect to other trace impurities (particulate matter, sulfur dioxide, nitrogen oxides) in the flue gas that can degrade sorbents and reduce the effectiveness of certain CO_2 capture processes;

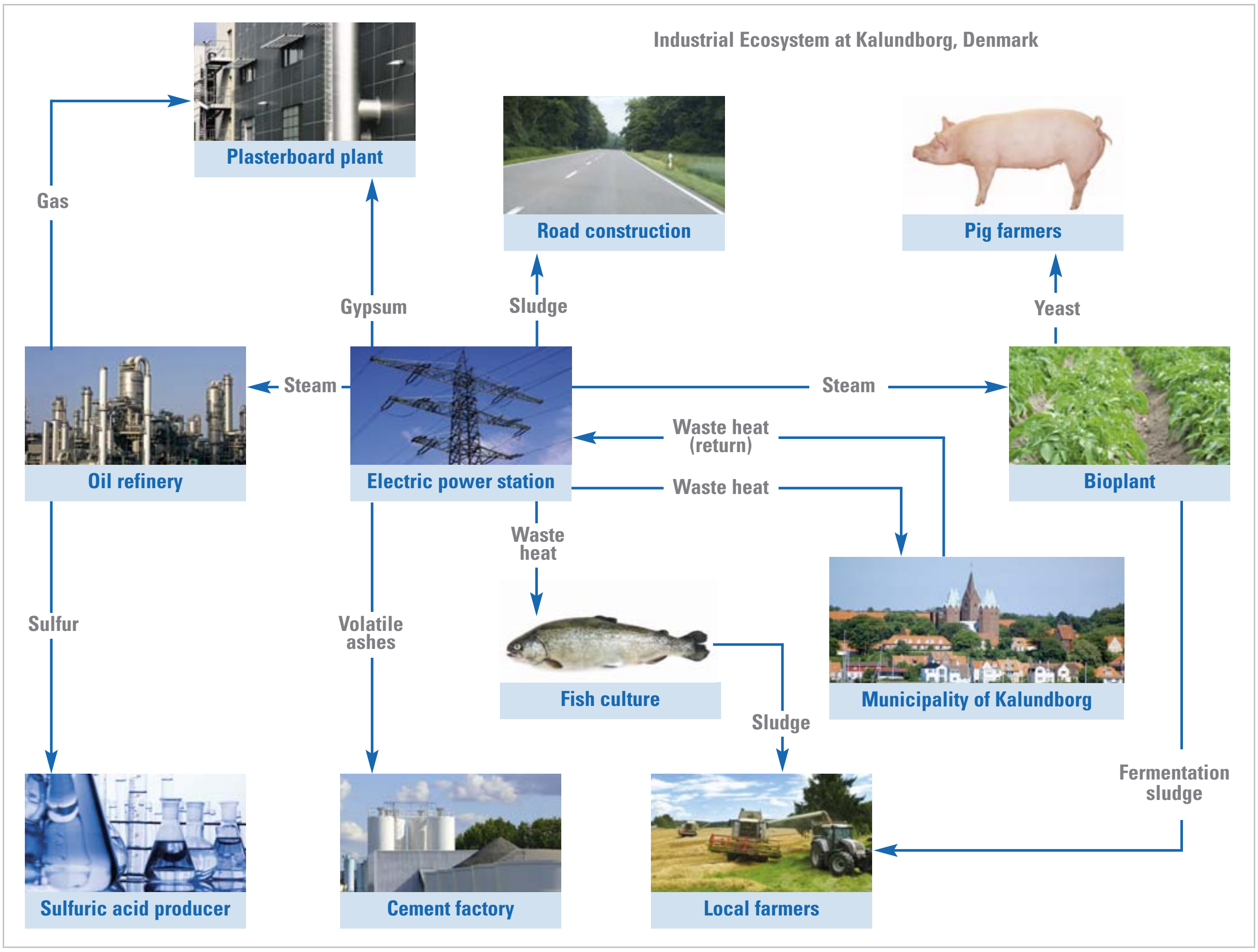

Fig. 5.9.5: Industrial ecosystem at Kalundborg, Denmark.

- Nanomembranes: self-organised and nanostructured membranes can help to improve efficiency and robustness of CO_2 capture, separation and storage;
- Use of energy efficient processes directly at the nanoscale, both to store and unstore CO_2 as needed.

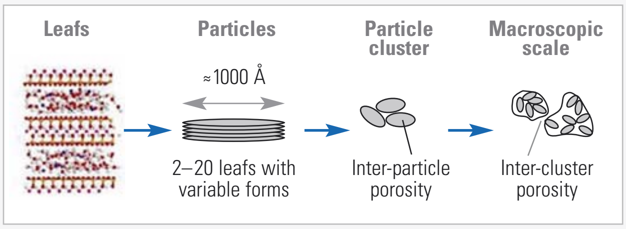

Fig. 5.9.6: The multi-scale spectrum of nanomaterials from nano- to macroscale.

- **CO_2 re-use**: New aspects should be regarded as potential new niches for CO_2 technologies :
  - Biomass management: using bio-inspired reduction (proteins/algae/enzymes) mechanisms that can be mimicked but synthetised catalysts stuck on specific surfaces/objects to enhance their efficiency for instance;
  - Catalytic and/or photolytic CO_2 reduction using photo/thermo/electro-assisted mechanisms;
  - Biocatalysts for CO_2 binding and reduction.
- **CO_2 sequestration**: nanomaterials can play a major role as a substrate for long-term sequestration and release: (NTC, chlatrates, alanates, bio-inspired sequestrations (sea, soil, biosphere), hard and soft matter.

Role of synchrotron radiation and neutron facilities

Accelerator-based x-ray and neutron facilities should play a major role for a better understanding of the microscopic and nanoscopic interactions between CO_2 and matter (hard and soft). Dedicated experimental set-up for nanodiffraction and nanospectroscopy should be built up for providing systematic data base of the CO_2 interaction at real materials under real conditions. The data base must the static and dynamic behaviour with respect to different structures, in the presence of water during O_2 interactions and combustion. Fundamental studies of thephoton/phonon/magnon interactions, under in-situ (pressure, temperature) conditions must be carried out in a comprehensive way.

This requires that dedicated instrumentation and equipment in support facilities must be made available for a direct access to the European research consortium responsible for this urgent matter.

Free Electron Laser facilities should be contacted to explore the possibility to implement instrumentation for real-time investigations of the CO_2-matter interaction process.

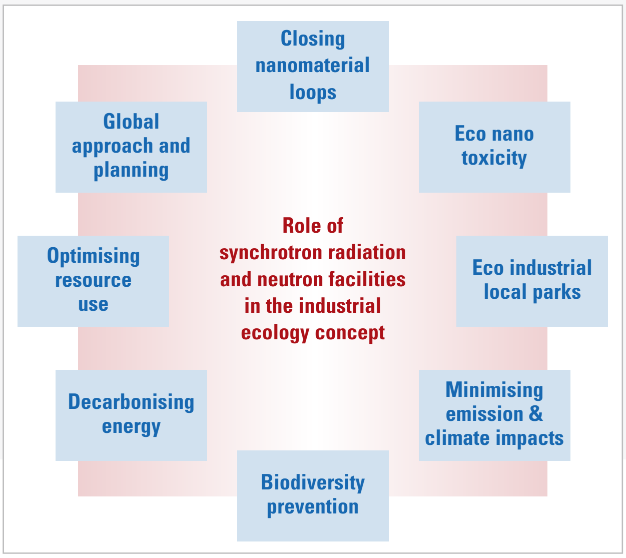

Fig. 5.9.7: The role of synchrotron radiation and neutron in the industrial ecology concept.

5.9.3. NUCLEAR WASTE

The safe geological disposal of the nuclear waste is one of the great scientific and technical challenges for 21st century's society. The demonstration that the corresponding issues can be technically solved with affordable methods is a key requirement to make nuclear energy production acceptable for society.

Since nuclear waste has to be isolated from the biosphere for thousands of years, a time span which cannot be covered experimentally, the prediction whether or not this is possible has to be based on very reliable models. It is evident that such critical predictions have to be based on a thorough understanding of the physical, chemical and biological processes, which control radionuclide migration from nuclear waste repositories. Various complementary approaches have to be performed for this purpose, involving different scales (from nanometres up to kilometres): laboratory experiments, characterisation of analogue system and finally, based on the data produced by these two approaches, modelling.

Migration processes depend critically on the type of waste produced. Current scenarios in Europe foresee the direct disposal of spent nuclear fuel (SNF) or of reprocessed waste forms. However, the waste forms may change with the advent of Fourth Generation reactor systems, which will be optimised to fulfil three major goals: (1) Increase the energy potential of stocks by converting and burning fertile materials by rapid neutrons and recycling the fuel; (2) Minimise the amount and the thermal load of waste to be disposed; (3) Reduce the lifetime and potential toxicity of waste by transmutation of major contributing elements on a long term time scale, followed by recycling in future reactors. It is evident that Fourth Generation systems will have a profound effect on nuclear fuel cycles and waste forms to be disposed of.

Nuclear energy actors know that it is necessary bringing waste management, their conditioning and storage in a continuous route of scientific and technological progress. This has been demonstrated in the past years, with significant results obtained in a better and better characterisation of waste, in a strong reduction of volumes and in the optimisation of the conditions of their implementation, conditioning and management.

Fuel recycling as an important step for reducing both quantities and radiotoxicity of waste has been chosen by some countries already many years ago. More significant progresses require a longer search along several axes, e.g. the reduction and quantity of nuclear waste at the time when they are produced, minor actinide separation and better conditioning in specific matrices. All these research directions aim at further reducing the quantity, the lifetime and finally the potential noxiousness of nuclear waste.

The minor actinides separation process aims at extracting long lifetime radionuclides. Some radionuclides, especially minor actinides, are eligible to be transmuted. This allows decreasing the amount of long term radioactivity. For other radionuclides, such as some long-lived fission products e.g. iodine as an example, transmutation will not bring significant results. Therefore, their conditioning in specific matrices tailored for a secure confinement, can be a progress route and an interesting research axis. Ceramic matrices are a promising solution and, in this domain, nanomaterials could bring a decisive breakthrough. Today this domain is a virgin area.

Another potential way to reduce the quantity of wastes on a very long time scale is the implementation of more efficient technologies for decontamination processes associated with the shutdown and dismantling of nuclear installations at the end of their life time. Innovative solutions may include for instance the replacement of washing solutions by surface active solutions (e.g. gels with reactive nanoparticles) or by nanostructured polymers capable of selectively fixing specific radionuclides.

All these research areas are found in a very long term roadmap on several decades time scale. Nuclear energy is a reality today. It produces very important quantities of energies which contribute to decrease greenhouse gas effects. It produces also nuclear waste which is already today, for the great majority, conditioned in matrices which guarantee a secure confinement (glass, concrete, bitumen). The reference solution for the long-live radwaste management chosen or envisaged by countries using nuclear energy is a deep geological repository. The demonstration of the feasibility of this solution has been made but it is necessary to reinforce these demonstrations.

The study of all of the processes relevant for nuclear waste disposal requires diverse scientific disciplines, ranging from material sciences to study corrosion processes of nuclear fuel, other waste forms and containers, to biogeochemistry and hydrology to follow the possible migration of radionuclides in the various parts of the repository system and the biosphere. Although macroscopic thermodynamic models have been developed to describe radionuclide migration, there are a number of key processes that have to be understood and quantified at the molecular level. In this context, nanoparticles and nanoscale processes constitute critical gaps in our ability to predict the perturbation induced by the nuclear waste disposal, particularly at the interface between the waste and engineered barriers

Combined with other methods as SIMS, EPMA, SEM and TEM, synchrotron radiation and neutron based methods, with spatial resolution in the micrometer and nanometer ranges, will greatly improve our knowledge of these nanoscale processes, permitting a reliable assessment of the risks associated with the long-term storage of nuclear waste, as well as the improvement of waste treatment procedures.

Nuclear waste and nanoscale processes

Spent nuclear fuel (SNF), with a worldwide inventory of 300,000 Mg, and HLW glass constitute the most significant part of radioactive waste. SNF consists predominantly of UO_2, while fission products (e.g. 129I, 131I, 137Cs, 90Sr), transuranium actinides produced by neutron capture and subsequent decay reactions (e.g. 239Pu, 237Np, 241Am) and activation products (e.g. 14C, 60Co, 63Ni), constitute only 3 to 4 atom percent. HLW glasses are homogeneous, alumino-borosilicate materials for the confinement of fission products and minor actinides after reprocessing of the SNF.

The probability of any release of radionuclides from SNF and glasses at deep underground repositories is minimised by placing multiple barriers between waste forms and the biosphere. Although the nature of these barriers varies depending on the country that developed it, a metallic container (copper, cast iron, low alloyed and/or stainless steel) is mostly envisaged as first technical barrier. Thus, alteration of both the barrier components and the waste forms, have to be studied in details. Key technologies for nuclear waste processes and long-term storage are closely associated to the capacity to predict the chemical durability and the mechanical behaviour of materials. During the iron or glass corrosion processes, interfaces (or interphases) made by the alteration products between the bulk material and the corroding media on a long timescale, are of special interest for future studies. Physico-chemical properties (thermodynamic stability, electrochemical reactivity, solubility, conductivity) of the phases constituting these interphases strongly depend on their structure and morphology at the nanometric scale (for example gel formed on altered glasses, barrier layers in metallic corrosion products etc). The behaviour of these interphases directly controls the global alteration kinetics of the material. Thus it is of primary importance to assess these phenomena using adapted investigation methods at different scales (i.e. current µ-XRD and µ-XAS, but also nanoprobes that will be developed in the future on synchrotron facilities and will allow performing these techniques on nano-volumes). These studies have to be performed on the one hand on samples simulating the long term alteration in laboratory and, on the other hand, on natural and archaeological analogues. These latter samples are the only possibility to study alteration layers formed on very long times in natural environments and to assess specific properties of the constitutive phases of the interfaces of interest.

Beyond the scale of the waste matrix, migration of radionuclides through confinement barriers is largely controlled by micro- and nanoscale processes (Fig.5.9.8). For example, argillaceous rocks are being studied as potential host rocks for nuclear waste repositories because to their very low permeability. In this type of rocks, migration of radionuclides is governed by diffusion and retention processes, which are both influenced at the nanometer scale by charged surfaces. Hence diffusion of radionuclides depends on their ionic form in solution. In clays with negatively charged surfaces, anions are subject to anionic exclusion which reduces the accessible porosity for diffusion, while cations are sorbed at the surface, which delays their migration. All these phenomena depend on the structure and texture of the rocks (porosity distribution, mineralogy). Therefore, in complement to macroscopic approaches, investigations from nm to mm scales should be used, by adapted methods, to identify and quantify the potential variability of transport parameters in a geological formation characterised by natural local heterogeneities:

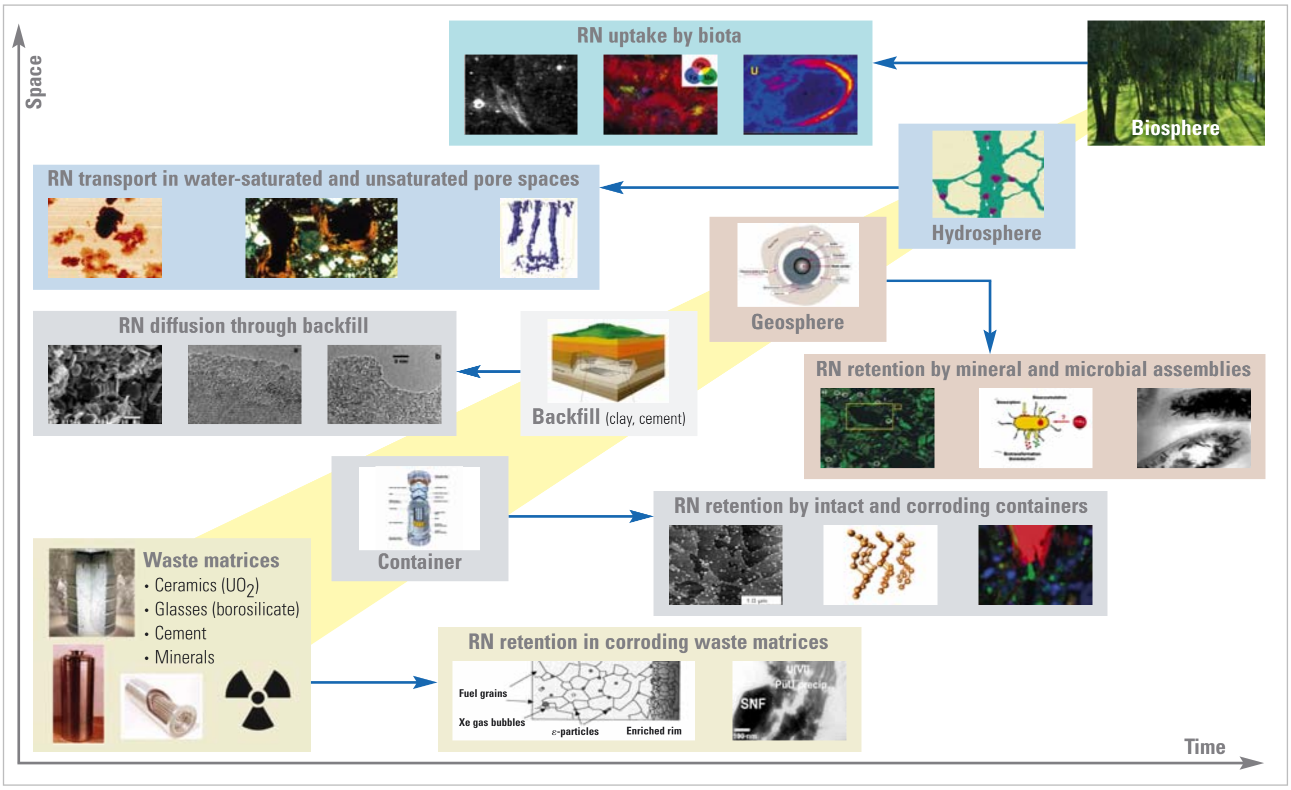

Fig. 5.9.8: Multiple barrier concept to reduce escape probability of radionuclides (RN) from deep geological waste repositories. Red arrows point to examples of relevant nanoscale processes.

- Internal processes in spent nuclear fuel and waste matrices:
  - Solid-state diffusion, formation of micro-fissures, gas diffusion, formation of corrosion layers at the SNF surface and at the cladding surface (Fig. 5.9.9);
  - Radiation damage in host phases for actinides and fission products.

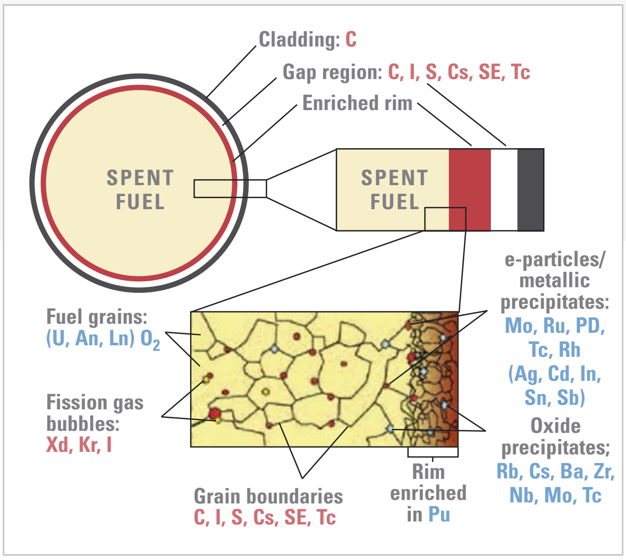

Fig. 5.9.9: Schematic representation of the microstructure of spent nuclear fuel. Both internal processes (self-irradiation, restructuration, solid-state and gaseous diffusion of radionuclides) and surface processes after contact with water (dissolution, corrosion, redox processes, radical and gas formation) are likely to be first controlled at the nanoscale. Courtesy: Mineralogical Society of America, Elements, December 2008.

- Surface processes of spent nuclear fuel and waste matrices:
  - Surface dissolution/corrosion/redox processes of SNF and after waste matrices under oxidising and reducing conditions (Fig. 5.9.9);
  - Colloid formation (Fig. 5.9.10);
  - Corrosion and mechanical failure of waste containers.

- Radionuclide migration in geomedia:
  - Backfill precipitation and diffusion processes;
  - Retention of radionuclides in multi-mineral and multi-organic environments dominated by chemical microdomains;
  - Retention by micro-organisms;
  - Colloid formation and migration (Fig. 5.9.10);
  - Solute transport.

- Radionuclide transfer along biomolecular interfaces:
  - Microorganisms;
  - Plants, soil-root transfer, internal translocation;
  - Animals and man, uptake by inhalation and ingestion, internal translocation.

- Analogue studies for investigation on long-term evolution and contribution to validation of long-term predictions (Fig. 5.9.11):
  - Natural nuclear reactors;
  - Uranium ore deposits;
  - Uranium mining sites;
  - Basaltic glass, Obsidian, Roman glass altered in various environments;
  - Archaeological corroded metallic artifacts.

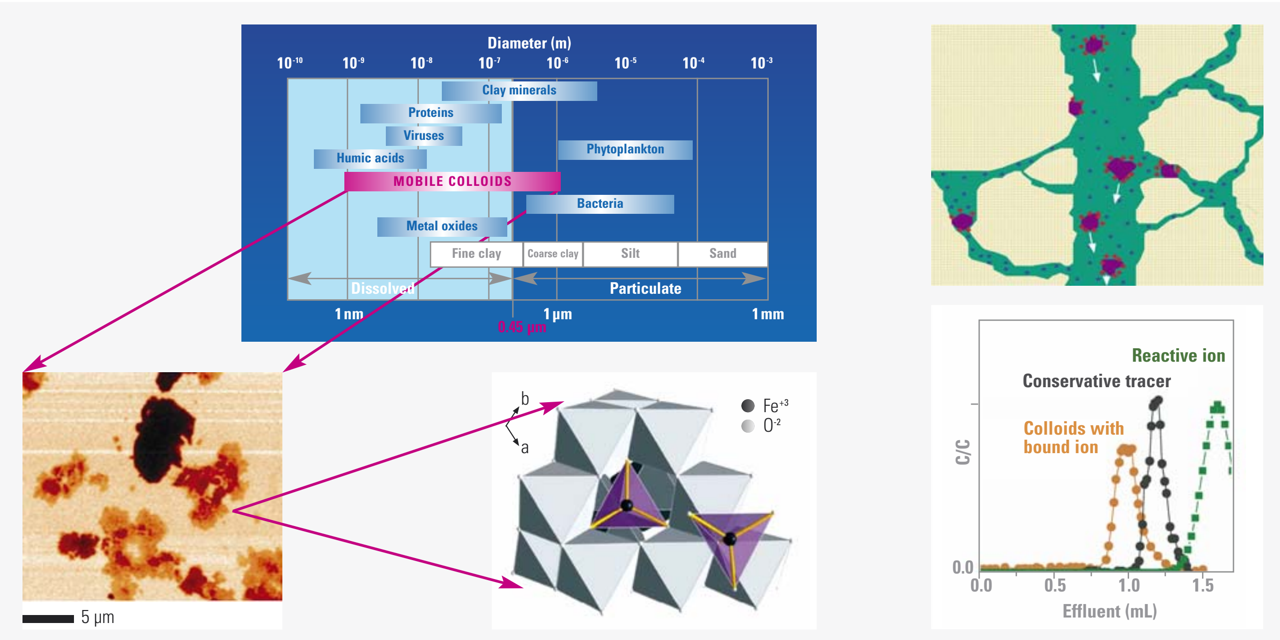

Fig. 5.9.10: Clusters and colloids play a major role for accelerated radionuclide transport through aquifers, as well as for their retardation. Although first results have been provided by neutron and synchrotron technique, major research breakthroughs are still restricted by limited spatial resolution on one hand, and by restricted access for radioactive samples on the other hand.

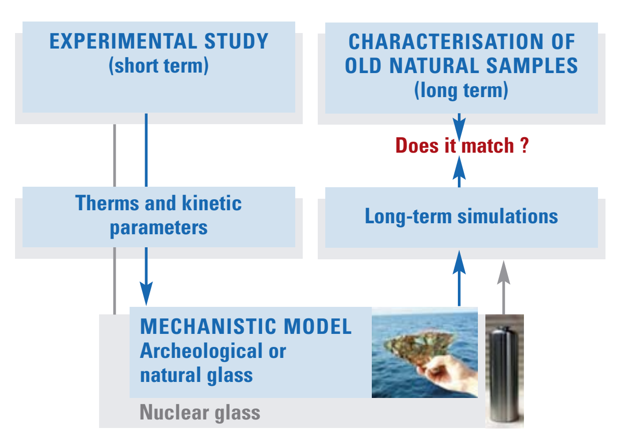

Fig. 5.9.11: Use of natural or archeological analogs to validate predictive models applied to the long-term behaviour of nuclear glass in geological repositories: example of glass alteration by water. In blue, studies conducted on natural or man made materials, in grey studies performed on nuclear glass. This approach has to be carried out for all the key phenomena expected to control the source term.

Research topics with synchrotron radiation and neutrons impact

Internal structure of spent nuclear fuel (SNF)

Nanoscale investigation of physical and chemical processes in nuclear fuel during and immediately after nuclear fuel burn-up leads to the development of fuels with higher efficiency and to improved direct disposal and reprocessing methods:

- Nanoscale solid-state phase separation processes in SNF;
- Formation of micro-fissures and gas diffusion;
- Chemical and physical properties of microdomains;
- Comparative investigation of different fuel types from 4th generation reactor designs (very-high-temperature, supercritical-water-cooled, lead-cooled fast reactors, thorium-based reactors);
- Migration of radionuclides into gaps between SNF and zircaloy cladding;
- Nanoscale redox processes (with intact zircaloy cladding);
- Structural and chemical characterisation of zircaloy cladding.

Synchrotron radiation and neutron facilities are needed for:

- 3-D investigation of pore structure in SNF (pore size distributions, continuity, tortuosity,...);
- Elemental and radionuclide separation in relation to nanoscale domains and gas voids;
- Identifying chemical form of fission products in SNF;
- Structure of crystalline and amorphous nanoscale domains;
- Interrogating oxidation states and other electronic properties of nanoscale domains;
- Short-range order of radionuclides in nanoscale domains.

Composition & structure of nuclear glass

Nanoscale investigation of physical and chemical constrains in nuclear glass are of primary importance in order to develop new materials matching with new nuclear waste:

- Nanoscale phase separation processes;
- Solubility of radionuclides depending on the glass composition and melting process;
- Formation of micro-fissures and gas diffusion;
- Chemical and physical properties of microdomains.

Synchrotron radiation and neutron facilities are needed for:

- Structure of amorphous glassy structure and crystalline nanoscale domains;
- Interrogating oxidation states and other electronic properties of nanoscale domains;
- Short-range order of radionuclides in nanoscale domains.

Corrosion of spent nuclear fuel (SNF)

The understanding of nanoscale corrosion processes is crucial for the development of the most efficient disposal systems, including container and engineered near-field barrier design:

- Surface dissolution processes and rate-limiting steps at nanoscale;
- Influence of different ligands;
- Redox processes at the SNF/groundwater interface under α,β,γ-radiolysis conditions and in presence of H_2 produced by container corrosion;
- Formation and dissolution of corrosion layers;
- Gas and ion diffusion through corrosion layers.

Synchrotron radiation and neutron facilities are needed for:

- Characterisation of stress and formation of fissures in zircaloy cladding;
- Molecular mechanisms of dissolution at SNF surface;
- Interrogate electron transfer processes at pristine and corroded surfaces in situ under oxic and anoxic conditions;
- Structural and chemical investigation of corrosion layers with nanoscale resolution;
- Radionuclide diffusion and retention through corrosion layers and disintegrating cladding.

Alteration of nuclear glass

The understanding of nanoscale alteration processes is crucial for the development of the most efficient disposal systems, including the container and the engineered near-field barrier design:

- Surface dissolution processes and rate-limiting steps at nanoscale;
- Influence of different ligands;
- Formation and dissolution of alteration layers;
- Water and ion diffusion through alteration layers.

Synchrotron radiation and neutron facilities are needed for:

- Characterisation of cracks formed after elaboration;
- Molecular mechanisms of glass dissolution;
- Structural and chemical investigation of alteration layers with nanoscale resolution;
- Water and ion diffusion through alteration layers;
- Radionuclide retention mechanisms in the glass alteration products.

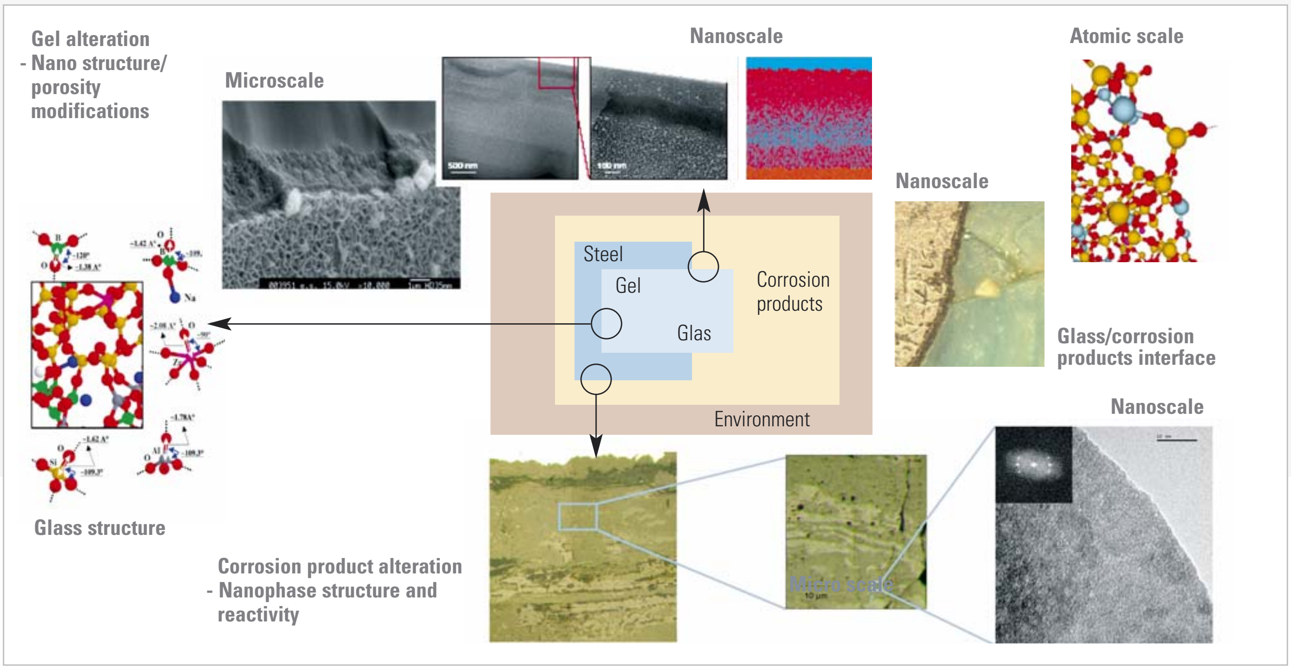

Fig. 5.9.12: Characterisation and modelling of interfaces at the micro, nano and atomic scales in the glass/steel/environment system.

Development of matrices for reprocessed SNF and transmutation

Nanosciences and -technology are crucial for the development of matrices which are resistant against radiation and dissolution in aqueous environments, properties relevant both for transmutation and the disposal of reprocessed nuclear waste:

- Investigation of α-radiation induced phase transitions, nanoscale phase separation and clustering, and amorphisation of crystalline matrices (pyrochlores, zircon, phosphates, …);
- Alpha-radiation induced changes in glasses;
- Secondary phase formation and interaction with radionuclides;
- Influence of oxidising and reducing conditions on solubility.

Synchrotron radiation and neutron facilities are needed for:

- Visualisation of nanoscale structures and chemical microdomains in matrices;
- Investigation of nanoscale phase transition and amorphisation processes in different matrices under alpha-radiation;
- Nanoscale surface dissolution processes as a function of time/doses;
- Surface redox processes under oxidising and reducing conditions
- Identification of secondary phases.

Development of containers for high-level nuclear waste and long term corrosion modelling

Containers are one of the first technical barriers to separate high-level nuclear waste from the environment. Nanosciences are crucial to improve their mechanical and chemical strength and to study radionuclide retention mechanisms in case of a failure:

- Behaviour of container walls under realistic disposal conditions: influence of internal and external pressure build-up, temperature, aggressive gases and fluids, gamma and neutron radiation;
- Corrosion processes under oxic and reducing conditions;
- Radionuclide migration through micro-fissures and corrosion rims;
- Redox processes at both metallic and corroded container walls.

Synchrotron radiation and neutron facilities are needed for:

- Nanoscale investigation of the pristine containers with special emphasis on the structurally critical points (welding and closure points);
- Nanoscale structure investigation of container walls after exposure under typical disposal conditions;
- In-situ investigation of corrosion processes;
- Chemical and physical characterisation of corrosion products;
- Molecular-scale interaction processes of radionuclides on metallic and oxidised container walls;
- Electron transfer reactions at corrosion rims and redox interactions with radionuclides;
- Nanoscale characterisation of radionuclide eigencolloids and of metal oxide and sulfide colloids with binding capacity for radionuclides.

Development of efficient backfill materials

Backfill is required to restrict water and gas diffusion and to reduce mechanical stress of containers. Nanosciences are required to study the microporous structure and transport processes:

- Investigation of porosity of various materials under realistic waste storage conditions;

- Study of the potential buffer material alteration processes due to the contact with container materials;
- Investigation of diffusion of water, dissolved and colloidal or colloid-bound radionuclides, and gaseous radionuclides through backfill materials to select the most suited materials, conditioning and packing procedures.

Synchrotron radiation and neutron facilities are needed for:
- Nano- and microscale tomography to study pore-size distribution, pore shapes, continuity and tortuosity;
- Molecular-scale investigation of radionuclide sorption reactions;
- Molecular scale study of buffer alteration processes]
- In-situ investigation of dissolved and colloidal radionuclide transport processes through backfill.

Radionuclide migration processes in the geosphere and hydrosphere

The geologic matrix surrounding nuclear waste consisting of e.g. granitic bed rock, clay deposits or rock salt, is intrinsically heterogenous at many scales, including the nanoscale.
- Multiscale porosity to predict water, solute and colloid transport;
- Multi-scale chemical heterogeneity and influence on radionuclide adsorption/desorption, oxidation/reduction and precipitation/dissolution processes;
- Multi-scale biological heterogeneity (distribution and structural self-organisation of microorganism communities in pore spaces) and influence on radionuclide adsorption/desorption, oxidation/reduction and precipitation/dissolution processes;
- Colloid formation and migration with groundwater.

Synchrotron radiation and neutron facilities are needed for:
- Investigation of 3-D pore networks in sediments and rocks (pore size distributions, continuity, tortuosity);
- Investigation of the mineral distribution with focus on nanominerals;
- Investigation of microbial distribution;
- Radionuclide distribution among minerals and micro-organisms with focus on nanoscale soil-water interfaces controlling radionuclide transport;
- Chemical speciation at controlling interfaces;
- Structural and chemical characterisation of colloids (RN eigen-colloids and RN sorbed to metal oxide colloids).

Radionuclide migration processes in the biosphere

Radionuclide distribution in the biosphere involves transfer into plants, the food chain, and ultimately to man. Nanoscale processes control RN at many interfaces.
- Radionuclide transfer from soil to plant roots;
- Influence of microbial and mycorrhizal interfaces;
- Translocation from roots to stem, leaves and reproductive plant organs;
- Uptake by animals and man through the food chain.

Synchrotron radiation and neutron facilities are needed for:
- Spatial distribution and chemical speciation of radionuclides at water/soil/root interfaces;
- Spatial distribution and chemical speciation of radionuclides in transport vessels (xylem, phloem) and cell organelles of vascular plants;
- Spatial distribution and chemical speciation of radionuclides along mucous membranes, blood vessels, organs of mammals.

Analogue studies

Natural nuclear reactors and uranium deposits with ages up to 2000 millions years provide insight into the long-term behavior of radionuclides in a range of geological conditions relevant for engineered underground disposal facilities and the surrounding geosphere.
- Radionuclide retention and migration mechanisms in relation to reconstructed ages, hydrology and geochemistry;
- Comparison with processes in comparatively young uranium mine tailings;
- Multiscale porosity, mineral and microorganism distributions and their relation to radionuclide adsorption/desorption, oxidation/reduction and precipitation/dissolution processes.

Natural and archeological glasses altered in various environments allow the validation of predictive models:
- Alteration mechanisms and reaction kinetics depending on the thermal, chemical and physical parameters;
- Radionuclide retention in the alteration products.

Synchrotron radiation and neutron facilities are needed for:
- Requirements are essentially identical to those previously given in the section related to nuclear glass alteration.

Conclusions

- Understanding the fundamental processes in nuclear waste repositories with unprecedented detail is a key requirement for assessing a final solution for nuclear waste treatment, and ultimately for the acceptability of nuclear energy by society.

- Still open questions are related to nanoscale processes, including the behaviour of ceramics and other nuclear waste forms under self-irradiation, redox and dissolution processes at waste container/water interfaces, the transport of dissolved and colloidal radionuclides in natural geomedia characterised by chemical microdomains, and biomolecular interfaces controlling transfer of radionuclides to microorganisms, plants, animals and man.

- Investigation of these nanoscale processes requires a range of synchrotron and neutron techniques with micrometer to nanometer resolution (Table 5.9.1). Note that moving from the state-of-the-art (15 nm for few techniques) to below 7 nm will have a great impact and then from there down to 2 nm and possibly to the subnanometre level once again. At the same time, larger scales up to the millimetre and decimetre range should not be neglected in order to tie in (chemical) molecular processes with (physical) transport processes.

- X-ray microscopes with lower to subnanometre resolution for chemical 2-D and 3-D imaging;
- Tunable x-ray beams (0.1 to 35 keV and beyond) with variable spot-size (<nanometre) and high photon flux (>1012 ph/s) to perform chemical speciation of all relevant elements with high spatial resolution;
- X-ray emission including RIXS spectroscopy to study redox processes;
- X-ray 3-D tomography with chemical information (energy tunable), nanometre to millimetre resolution and large sample sizes (dm);
- XRD with (sub)nanometre spatial resolution;
- HEXS: high-energy x-ray scattering PDF of nanominerals, colloids, and dissolved clusters and complexes;
- SAXS and SANS: particle size distributions during nucleation of nanominerals;
- Neutron scattering techniques for non-crystalline aqueous systems, films etc. (isotopic replacement used to enhance contrast of particular atomic species);
- Surface scattering and glancing incidence XAS techniques, including GIXAS, crystal truncation rod diffraction, and long-period x-ray standing wave fluorescence, to study surface processes;
- Energy-dispersive XAS, time-resolved XAS and time-of-flight neutron techniques to study kinetics with sub-second temporal resolution.

Table 5.9.1: Select synchrotron and neutron techniques required for nuclear waste nanosciences.

- These techniques have to be accessible for highly radioactive and radiotoxic samples, including spent nuclear fuel and samples containing radionuclides with proliferation concerns (e.g. Pu-239). This requires beam lines and sample preparation labs with the respective safety installations, as well as the appropriate permissions and administrative regulations. Note that the SNF problem is an essential and driving part of the entire nuclear fuel cycle, but is barely accessible with current restrictions.

- These techniques have to be integrated with theory, simulation, and computational approaches and be linked to the macroscopic approach in order to ensure the consistency between the various scales.

- The research covers a wide range of different scientific fields, including nuclear chemistry and material sciences for the study of SNF and waste matrices, all aspects of environmental sciences including colloid and geochemistry, hydrology and soil physics and chemistry, several aspects of life sciences including biophysics and -chemistry, microbiology, plant physiology and medicine, beamline development and theory. Strong collaborative efforts between scientists of these different fields are essential for a multi-disciplinary approach.

- To make best use of synergies, this effort has to implement, utilise and build on already existing research infrastructures, e.g. national and international nuclear facilities and universities, as well as large-scale facilities.

EUROPEAN CENTRE FOR NUCLEAR WASTE RESEARCH AT SYNCHROTRON AND NEUTRON FACILITIES

Understand/control the nanoscale processes relevant for nuclear waste containement

Develop synergies between the different scientific fields involved in nuclear waste and the larges-scale facilities

Provide instrumental and administrative conditions to prepare and **measure radioactive** samples

- **Radionuclide** sample preparation labs
- **Radionuclide** synchrotron beam lines
- **Radionuclide** neutron beam lines

- Irradiation-induced chemical, structural and physical reorganisation of waste matrices and claddings
- Corrosion and dissolution of waste matrices
- Abiotic redox processes at surface of waste matrices and claddings
- Diffusion processes through waste matrices and man-made barriers
- Colloid formation and migration
- Microbial sorption, redox, mineralisation by structured microbial communities
- Abiotic sorption, redox and mineralisation in structured multi-mineral and multi-organic environments
- Solute transport through fractal pore spaces
- Water/soil/root interfacial processes
- Translocation processes in plants
- Uptake and translocation processes in mammals

Multi-disciplinary approach:

- Nuclear chemistry and material sciences

Environmental sciences:
- Geochemistry, hydrology

Life sciences:
- Microbiology, plant, physiology, medicine, physics (beam line development)

Coordination of joint research programs to provide access of external groups to European research infrastructures

Partnerships:
- Universities
- National and international nuclear research centres
- Nuclear industry with large scientific centres

Training:
- **Students and scientists**

Fig. 5.9.13: European Centre for Nuclear Waste Research.

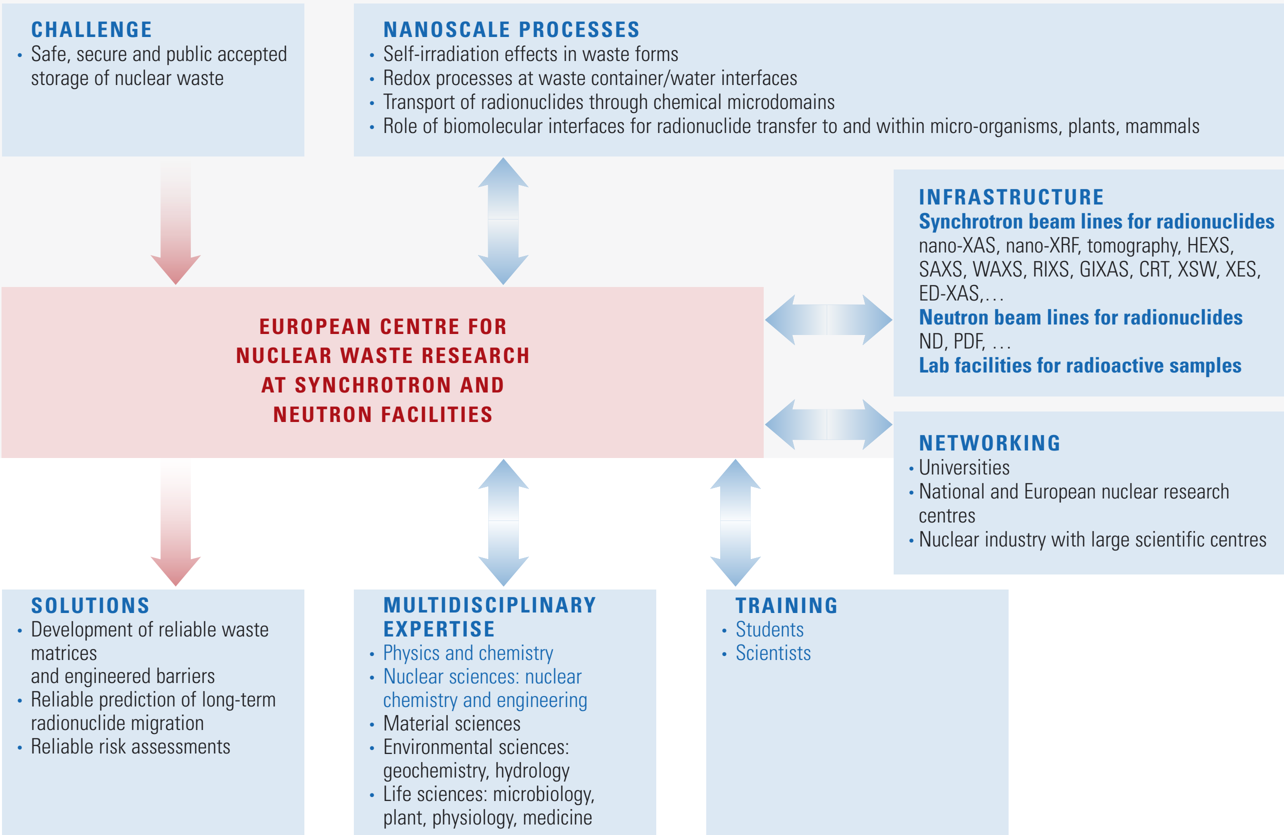

Fig. 5.9.14: European Centre for Nuclear Waste Research.

- These diverse requirements could be met more rapidly and much more effectively by establishing a European Centre for Nanoscale Nuclear Waste Research. It should be conveniently placed nearby a (already existing) neutron and synchrotron facility.

- With this new centre, multiple research breakthroughs towards the development of safe waste storage materials and procedures and towards reliable long-term risk assessments are achievable.

5.9.4. NANOPARTICLES IN THE ATMOSPHERE AND CLIMATE CHANGE

The earth's atmosphere consists of a gas phase in which nano- to micrometre scale particles ("aerosols") are suspended. They texture the atmosphere by providing solid or liquid surfaces and phases throughout the atmosphere, triggering:

- Condensation processes;
- Nucleation processes;
- Ionic-chemical reactions;
- Surface reactions;
- Scattering and absorption of sunlight;
- Water-cloud formation, and
- Ice formation.

These processes, in turn, affect air quality, human health and climate (see Fig. 5.9.15 and Fig. 5.9.16).

- **Role of nanoparticles for air quality**

The change in the composition of the troposphere is related to the increasing world population and its growing demand for energy, food and living space. These demands are associated with growing industrialisation and urbanisation, developing megacities, increasing traffic, and general land-use change. Increasing and changing emissions of primary trace gases and particles into the troposphere impact atmospheric chemical processes which control the removal of greenhouse gases and pollutants from the atmosphere (atmospheric self-cleaning), but also the chemical formation of new pollutants in the atmosphere such as ozone or secondary organic aerosols (SOA). It is expected that the trend in atmospheric composition change will lead to significant climate changes with detrimental effects on large parts of the world population.

The effect of pollution on mortality is shown in Fig.5.9.17. The aerosol particles can be efficiently deposited throughout the human respiratory system, particularly deep in the lung aioli at the air/blood interface. Therefore these particles may be harmful due to their mere presence, even if the substance is non-toxic.

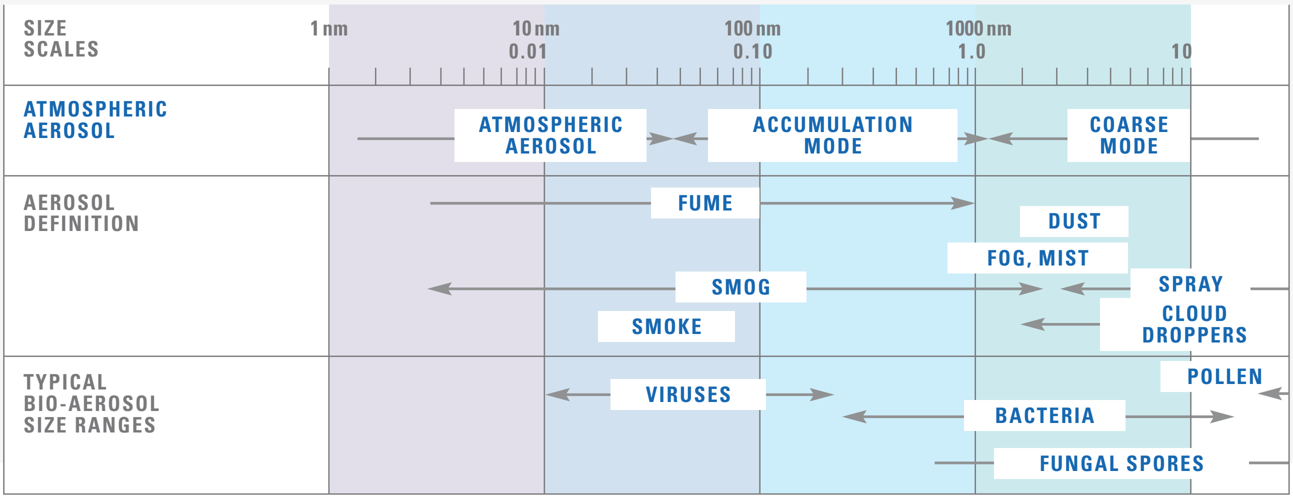

Fig. 5.9.15: Size, shape and composition of aerosols in the atmosphere.

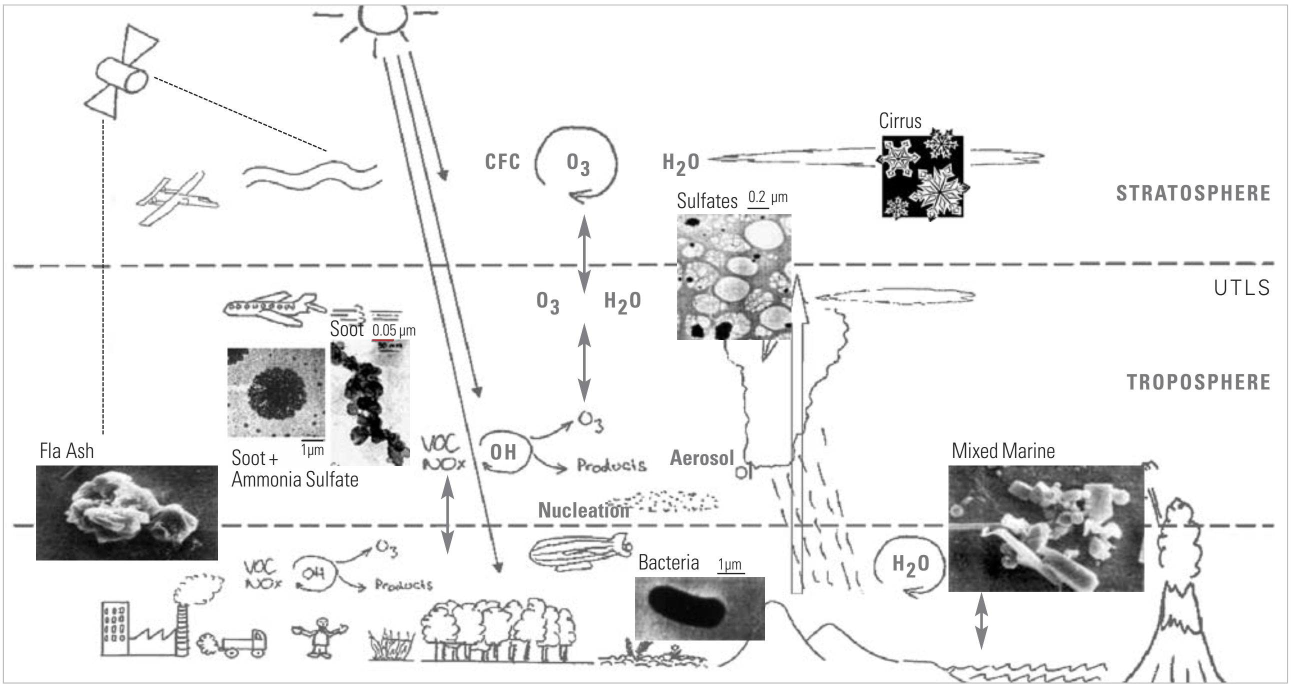

Fig. 5.9.16: Overview of atmospheric nanoparticles.

- **Role of nanoparticles for climate change**

The tropospheric chemistry and transport processes involved in atmospheric composition change occur on relatively short time scales (from minutes to years), thus resulting in a fast transformation and distribution of local anthropogenic and biogenic emitted trace substances over regional and global scales. In addition, increasing temperatures are expected to enhance the biogenic emission of reactive organic trace gases, which are the main precursors of photochemically formed organic aerosols. Two key attributes distinguish the impact of aerosol on climate compared to greenhouse gases. Due to the fact that aerosols accumulate in the sub micron size range and is resonant both with the wavelength of solar radiation and the Kelvin effect, (which controls the formation of cloud droplets), the radioactive impact of molecules condensed in aerosol particles on climate is amplified by about 1000 compared to molecules that remain in the gas phase. Furthermore, because aerosol particles have an atmospheric lifetime of a month, any changes in aerosol loading (anthropogenic or otherwise) have an immediate impact on climate, in contrast to the century time scale of long-lived greenhouse gases.

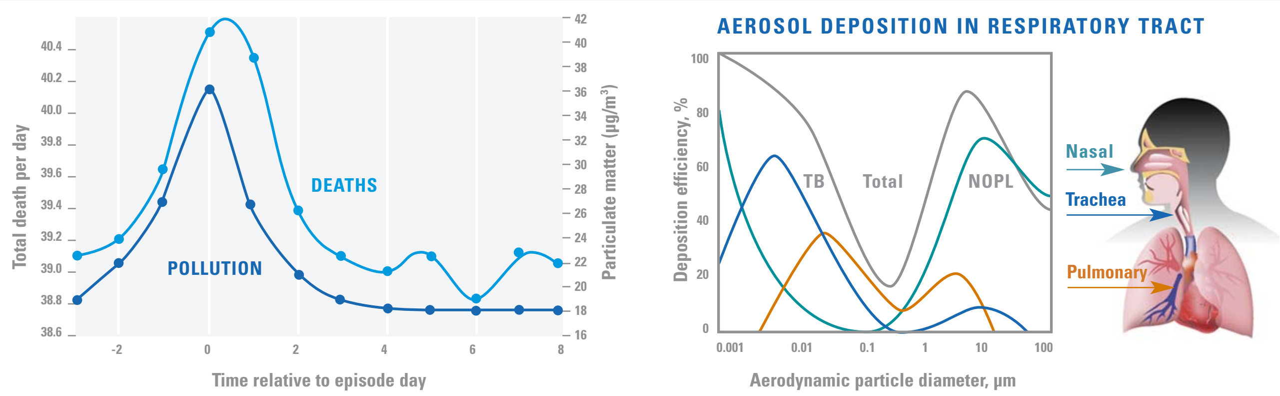

Fig. 5.9.17: Particle loading in pollution related to mortality. On the right: Aerosol deposition in respiratory tract.

The irradiative cooling effect induced by nano- and micrometre scale particles is currently the most important process for counteracting the warming induced by IR radiation absorbed by gas phase greenhouse gases (CO_2, CH_4, O_3, etc.). The physical and chemical state and processes of nanoparticles in the atmosphere have yet to be understood (see Figs. 5.9.18 and 5.9.19).

The challenge for atmospheric science and climate science is to provide an understanding of the relation between climate, air quality, and possible feedbacks within the Earth system. An understanding of the interaction between aerosol chemistry and its respective microphysical properties is necessary in order to produce reliable predictions of the effects of aerosol on the earth's climate as well as on health. This understanding is needed to assess the impact of natural and man-induced change on the global atmosphere and to contribute to the development of political tools that enable a sustainable society.

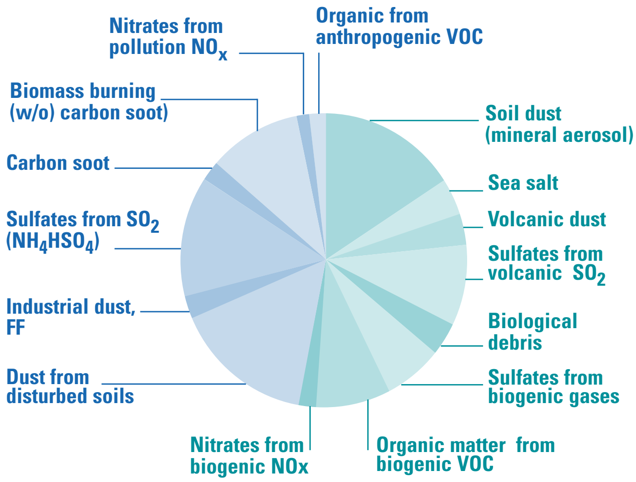

Fig. 5.9.19: Approx. anthropogenic and natural contribution to the global aerosol burden (< 2 nm diameter).

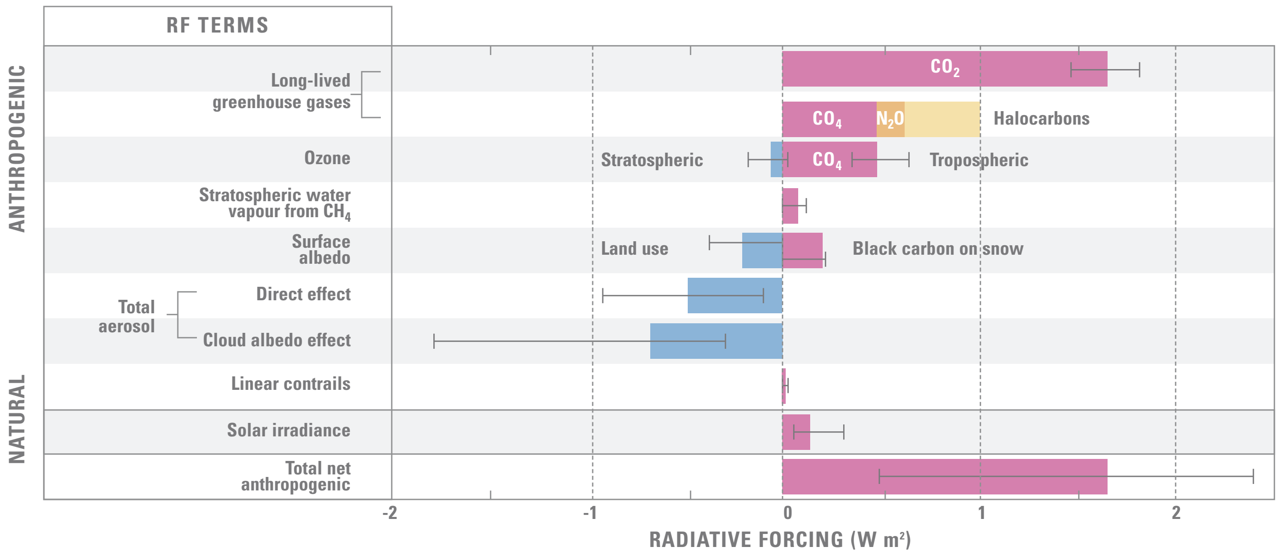

Fig. 5.9.18: Global-average radiative forcing estimates and ranges between 1750 and 2005. Negative radiative forcing results in cooling, positive in warming. Large error bars (uncertainties) for the effect of nanoparticles.

- **Nanoparticles and atmospheric and climatic processes**

Aerosol plays a key role in many key processes which determine the conditions for life on earth (see Fig. 5.9.20).

(a) Atmospheric chemistry:

- Polar stratospheric clouds (PSC) and their surface structure play a key role in the formation of the ozone hole by catalysis of the heterogeneous reactions which lead to ozone degradation;
- Multiphase chemistry: $SO_2 \rightarrow H_2SO_4$ oxidation in clouds;
- Heterogeneous chemistry: HONO, N_2O_5 on aqueous surfaces;
- Partitioning/oligomerisation of semi-volatiles which leads to removal of trace substances from atmosphere;
- Heterogeneous reactions modify the aerosol mass and its hygroscopic properties and affect the gas phase chemistry in the atmosphere;
- Ageing of aerosols and their ability to act as cloud condensation nuclei (CCN).

(b) Radiation balance:

- Direct effect: light scattering from clouds;
- Indirect effect: lifetime, precipitation, albedo of clouds;
- Semi-direct effect: light absorption, lifetime of clouds, radioactive properties of cirrus clouds, their microphysics properties, and the chemical and physical properties of ice nuclei particles;
- Contrail formation by aircraft emitted particles and their impact on cirrus (ice particle) formation.

(c) Biogeochemical cycles:

- Nucleation of new particles: biogenic versus anthropogenic;
- Combustion: biomass burning versus internal combustion;
- Via clouds: radiation and rain;
- Direct deposition and modification of atmospheric lifetimes;
- Fertilisation of nutrient poor eco-systems via deposition.

(d) Health and quality of life:

- Mobility of non-fluid substances;
- Traffic, condensed aromatics, PAH;
- Respiratory deposition;
- Visibility;
- EU limits for particle concentrations in cities (soot).

- **Research barriers**

Significant gaps in our understanding of the interaction between aerosol chemistry and microphysical properties of aerosols hinder reliable predictions on the effects of aerosols on climate and health. This applies especially to the secondary organic aerosol components (SOA) (see Fig. 5.9.21).

- Formation processes of organic particles (dependent on number and mass concentration), including higher order oxidation processes as inherent source of organic particles;
- Transformation processes during the atmospheric lifetime of organic particles;
- Chemical aging of particles by changing climate relevant optical, hygroscopic and CCN properties;

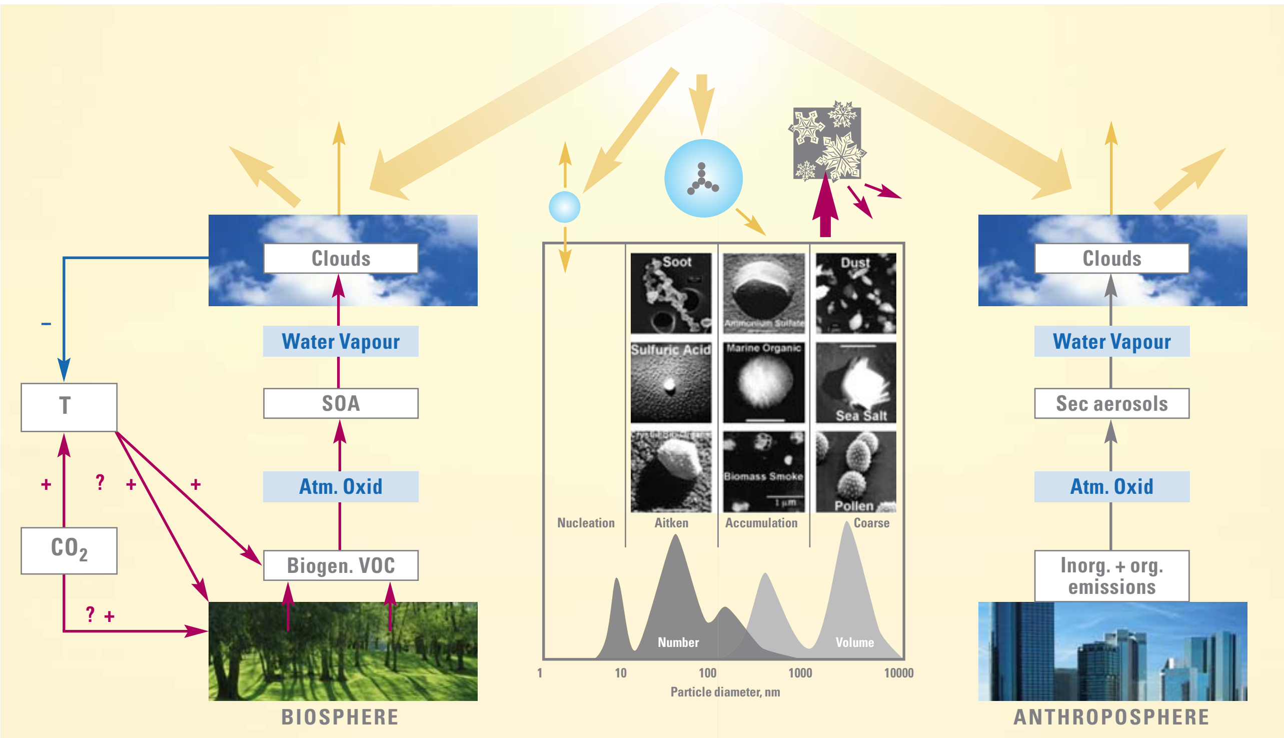

Fig. 5.9.20: Role of nanoparticles in atmosphere.

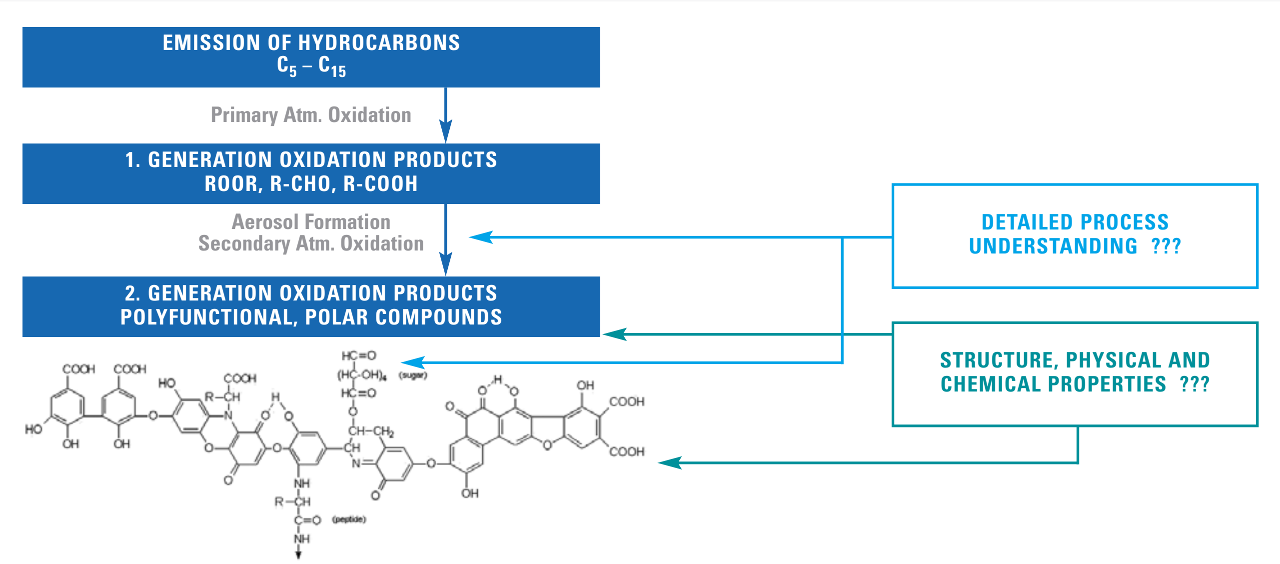

Fig. 5.9.21: Typical reaction mechanism for aerosol formation.

- Interaction of semi-volatile oxidised vapours and particulates during the aging process and its importance for the mass balance and the atmospheric cycle of reactive carbon;
- Separation and interaction of aerosol components arising from anthropogenic activities (e.g., energy production) and those originating from biogenic sources (e.g., vegetation);
- Coupling of primary emission of condensed organics from traffic, evaporation under dilution in the atmosphere, and subsequent recondensation of their oxidation products as SOA;
- Feedback between global warming, biogenic emissions and biogenic particle formation;
- Importance of cloud chemistry with respect to organic mass production, compared to other processes, has yet to be determined;
- Feedback between natural or anthropogenic land use change, aerosol formation and global warming.

- **Key priorities for fundamental research**

Analysis, physical and chemical identification of atmospheric nanoparticles and their transformation processes are of prime importance for the future understanding of atmospheric chemistry climate interaction:

- Understanding of formation processes of low volatility oligomers and polymers which may lead to significant changes in the current SOA modelling approaches;
- Identifying additional atmospheric trace gases as aerosol precursors which can contribute significantly to the currently underestimated SOA mass in the atmosphere by models;
- Aqueous phase chemistry – cloud processing of aerosols as a possible important source of SOA needs to be quantified;
- Chemistry and photochemistry of atmospheric aerosol aging and its impact on morphology and mixing state, and on aerosol – climate interaction;
- The coating process of black carbon (BC) by SOA, which can increase the single scattering albedo and the absorption cross-section of the soot particles, needs to be quantified under atmospheric conditions and to be considered in climate forcing studies;
- Better understanding of the biological activity of primary organic nanoparticles in the ocean;
- Characterisation of multicomponent aerosols and the internal mixing of aerosols;
- Quantification of the hygroscopic behaviour of different internally mixed aerosols for different humidities and temperatures and its effect on light absorption and light scattering properties and on the formation of CCN;
- Advanced characterisation of the chemical composition of organic (carbonaceous) aerosols, thereby avoiding artefacts in sampling and analysis of OA compounds;
- Incorporation of the direct (optical properties) and indirect effect (CCN activity) of organic aerosol in global climate models.

Role of synchrotron radiation and neutron facilities

Advanced analytical tools provided at modern European synchrotron radiation and neutron facilities must be exploited in order to achieve a better microscopic understanding of the physical and chemical atmospheric processes which are triggered by aerosols. This requires dedicated experimental set-ups, which allow studying the structure and behaviour of aerosols under relevant atmospheric conditions in a systematic way from the formation of aerosol precursors to the ageing of aerosols (see Fig. 5.9.22).

This includes:

- Nanodiffraction and scattering capabilities for individual aerosol particles in dedicated, atmospheric environments for multiphase aerosol;
- Nanospectroscopy and microscopy capabilities for individual aerosol particles at dedicated atmospheric and aqueous conditions;
- Real-time x-ray studies of chemical reactions on and within individual aerosol particles (as "black carbon coating") in combination

with optical light scattering and light absorption (FEL-optical laser instrumentation);
- Real-time studies of the formation process of aerosols (nucleation) and the characterisation of the aerosol surface (surface layers, enrichment of ions) and the morphology for single and multiphase aerosol;
- Quantitative neutron incoherent H scattering studies for monitoring water uptake by aerosols under real conditions and to obtain surface structural information;
- High-sensitivity nanotomography in absorption or fluorescence mode to determine 3-D chemical composition of aerosol under in-situ conditions;
- Ionisation via VUV radiation for molecular analysis of organic compounds via high resolution mass spectrometry;
- Development of dedicated beam lines and instrumentation which address the specific challenges of soft x-ray spectroscopy

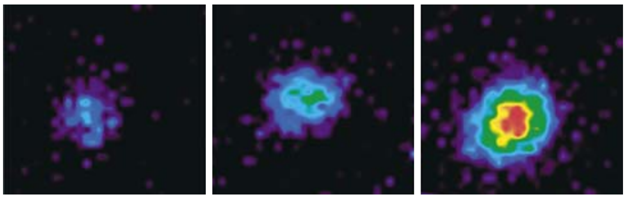

Fig. 5.9.22: Diesel passenger car particles after atmospheric photo-oxidation for several hours in a smog chamber. Scanning transmission x-ray images of a soot particle 200 nm in diameter at 30, 52 and 88% relative humidity. The pictures were taken at 538 eV, where oxygen absorbs due to a resonant transition. The absorption is a direct and in-situ probe of the increasing amount of water adsorbing to the soot particle with increasing humidity.

Conclusions and European research strategy

The European synchrotron radiation and neutron facilities must develop the appropriate analytical technologies which provide the necessary microscopic understanding of all physical and chemical processes which are related to the presence of aerosols in our atmosphere. A pan-European consortium on “Nanoscience Issues in the atmosphere and the earth's climate” must be implemented, which coordinates inter alia the analytical needs. Based on a strong interaction between the communities in atmospheric research and synchrotron radiation and neutron facilities important, climate relevant processes on the nanoscale will be quantified (see Fig. 5.9.23). This will be one of the cornerstones for scientific advice for society and politics with regard to:

- Interaction/competition of nucleation and combustion formation of particles;
- New diesel, aircraft engine technologies – understanding smaller and smaller particles;
- Optimisation of the transport sector relative to the environment (hybrid cars, aircraft engines, better fuel);
- Natural vs industrialised atmosphere; past, present, future;
- Future climate scenarios;
- Regional, global mitigation/adaption options;
- Testing the validity of climate geo-engineering suggestions.

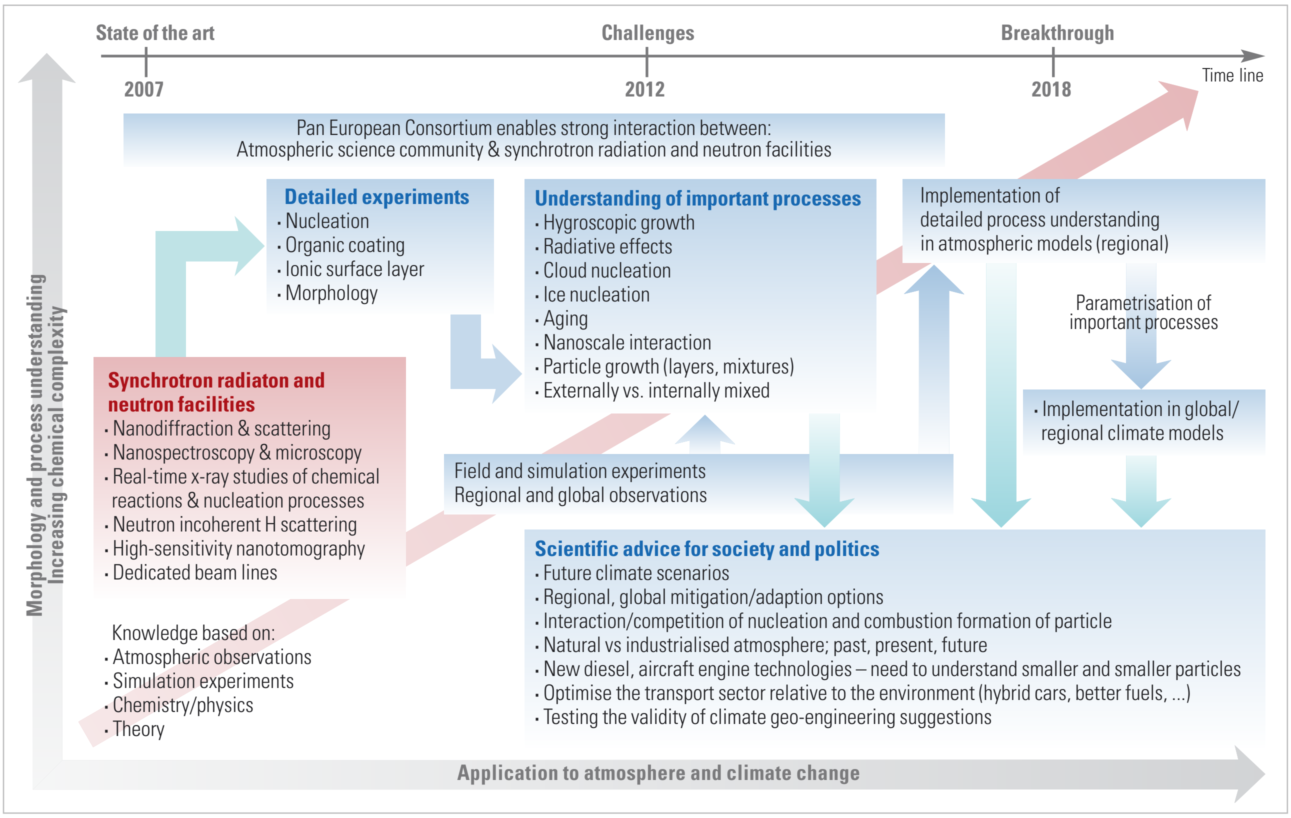

Fig. 5.9.23: Roadmap for future research on nanoparticles in the atmosphere.

5.10. TOXICOLOGY

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[Affiliations chapter 12]

Definition

Approximately 400 manufacturer-identified nanotechnology-based consumer products are now on the market. By assembly of atoms and molecules to form substances and devices, the size-dependent properties of nanoscale materials for applications ranging from cosmetics to fuel cells is reaching the mass market at increasing numbers and amounts. Yet our understanding of the potential toxicity of nanoparticles remains rudimentary. To determine whether the unique chemical and physical properties of new nanoparticles result in specific toxicological properties, the nanotechnology community will need new ways of evaluating hazard and ultimately assessing risk.

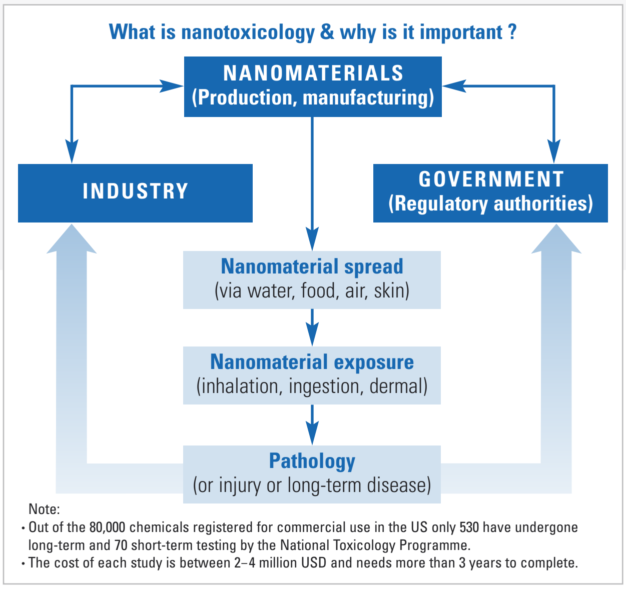

Fig. 5.10.1: Overview of nanomaterials for toxicology.

Nanotoxicology research needs

Critical information is still needed to understand the human health impact of nanoparticles and help define the mechanisms responsible for any adverse effect.

- Nanoparticle toxicity will need to be systematically explored and the variety of nanoparticle characteristics that act as key factors that determine toxicity responses and profiles will need to be determined;
- Extensive nanoparticle physicochemical characterisation is needed, including particle size, size distribution, shape, surface area (some proposed specifying bio- available surface area), redox potential and properties, purity/identity of contaminants, and catalytic activity, in addition to generation of reactive oxygen species;
- Nanomaterials must be characterised repeatedly in order to reflect their physicochemical state in relevant environmental media and their potential transformation at the portal of entry (e.g., the lung, skin, and gastrointestinal tract) and at the target organ. Therefore, new tools for in-situ characterisation of nanoparticles are necessary;

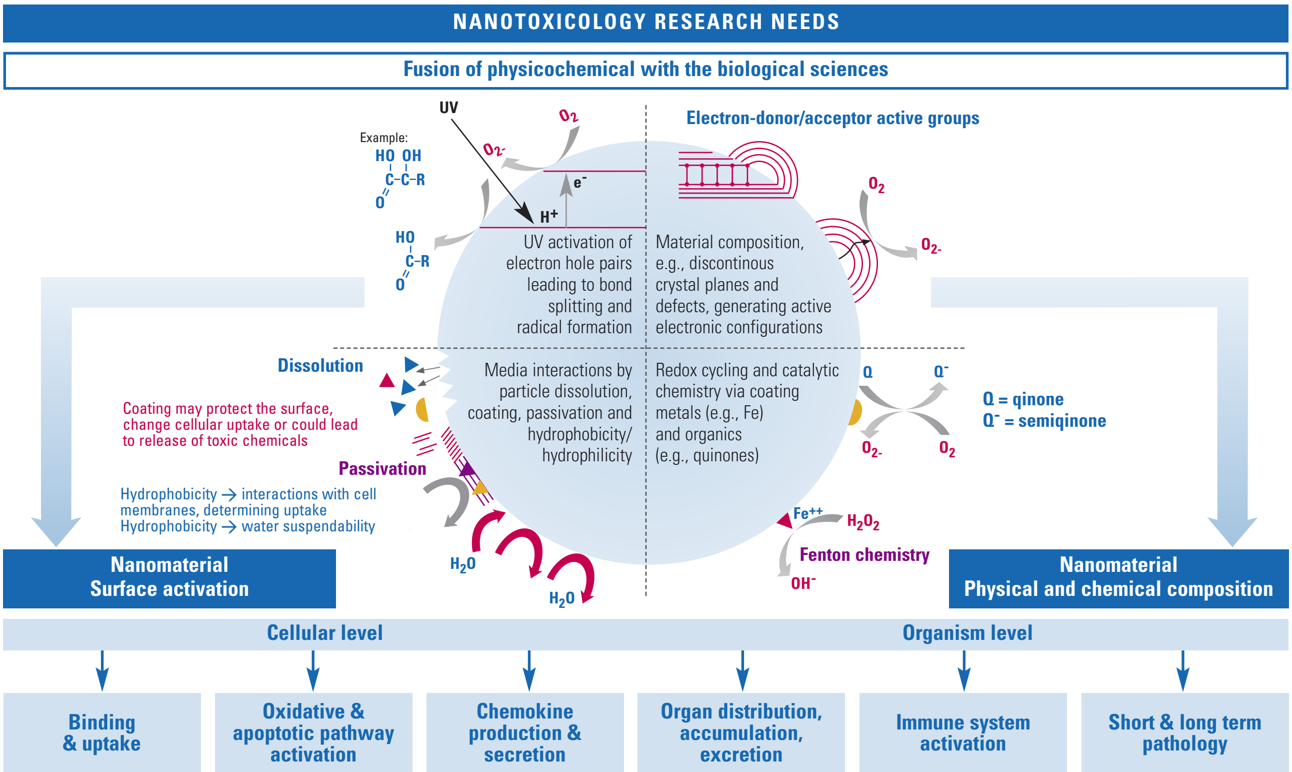

Fig. 5.10.2: Nanotoxicology research needs.

- Characterisation of the nanomaterial should be carried out for all phases of the product lifecycle during which exposure or release may be anticipated;
- Standardised protocols for nanoparticle characterisation will be essential to assure consistency across laboratories. Standards for nanoparticle characterisation and their correlation to toxicity responses should be developed;
- Determination of the degree to which nanoparticles interact with biological matter, including DNA, cytoskeletal structures, collagen, and membrane structures. Therefore, connections between the physical characterisation of nanoparticles must be established with the cellular biology of their interactions with cells and intracellualar components;
- Toxicokinetic studies are still scarce and will be needed to determine which nanoparticles will be detected by macrophages (in the lungs or other tissues) and whether they will consequently translocate into the systemic blood circulation. Detailed mechanistic correlations between nanoparticle composition and physicochemical properties and membrane translocation may reveal ways to "engineer out" the capacity for widespread distribution and subsequent toxicity through modification of surface coatings or other aspects of nanoparticles;
- Cross-disciplinary communication needs to be established. In-depth understanding of nanoparticle toxicology requires elucidation of the relationship between physicochemical parameters and mechanisms of toxicity, greater communication is needed between physical scientists (chemists, physicists) skilled in characterisation of materials and toxicologists, pharmacologists and biologists able to discern mechanisms for toxicity;
- Toxicology testing needs to be updated and become more holistic in order to be able to determine toxic responses and risks from new nanoparticles but in ethical and efficient ways. The role of new whole body imaging biomarkers as indicators of toxicokinetics and toxicological responses should be further developed. Also, use of molecular technologies, including toxicogenomics and proteomics, may be more efficient at identifying novel mechanisms of toxicity.

NANOMATERIAL PHYSICAL & CHEMICAL CHARACTERISATION PARAMETERS

Structural parameters
- Particle size/size distribution
- Agglomeration state/aggregation
- Shape
- Crystal structure
- Porosity

Surface parameters
- Overall composition (including chemical composition and crystal structure)
- Surface composition
- Purity (including levels of impurities)
- Surface area
- Surface chemistry, including reactivity, hydrophobicity
- Surface charge
- Interfacial energy
- Photocatalytic activity

Stability parameters
- Time-dependent (dynamic, stability)
- Storage, handling, preparation, delivery
- Solubility and the rate of material release through dissolution
- Aggregation state in different environments (buffers, biological tissues)

Dosimetry parameters
- Concentration-dependent dispersibility
- Dose-dependent effects on cell biology and physiology

Fig. 5.10.3: Nanomaterial physical and chemical characterisation parameters relevant to toxicology studies.

The importance of nanomaterials characterisation in nanotoxicology

It is common understanding among the toxicology and nanotechnology fields now that poor characterisation of a nanomaterial could cause irreparable damage to the entire field, and lead to missed opportunities that could benefit consumers and patients. The regulatory authorities and litigation attorneys may be biased or wrongly led by the conclusions of a single study, something that should be avoided given the limitation of any single study. Therefore, there is a great need for detailed systematic studies carried out or coordinated by a centralised body. The role and importance of physical and chemical characterisation studies of nanomaterials is generally considered the most important piece of information to be fed-in to allow the design of biological studies.

Synchrotron radiation and neutron facilities are needed for:
- Neutron reflectometry to determine surface characteristics of nanoparticles;
- SAXS/WAXS to determine the structure of nanoparticles and nanocomposites;
- Time resolved x-ray and neutron sources to help determine the toxicokinetic profiles of nanoparticles in the body;
- Kinetics of inhaled nanoparticles at the cellular and mucosal (e.g. nasal, alveolar) level;
- Large-scale facilities in collaboration with centralised bio-informatics facilities to help establish nanoparticle structure-genotoxicity assays;
- High-end Electron microscopy facilities to establish morphological and structural characteristics of nanoparticles;
- Interaction of electrons, neutrons and other radiation particles with nanoparticles and the effect on their structural characteristics;
- Electron and neutron based techniques in the determination of nanoparticles in the environment and the impact of their accumulation in the food chain.

5.11. ANCIENT AND HISTORICAL SYSTEMS

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[Affiliations chapter 12]

In archaeology, palaeontology, conservation sciences (cultural heritage) and palaeo-environment, the heterogeneity of the materials is a major barrier for our understanding. Key research questions related to the study of human and natural evolution and the safeguarding of our cultural heritage by gathering technological, cultural, biological and environmental information at the macro- to nanoscales. Typical open questions are:

- Effectiveness of new and old conservation treatments;
- Suitability of museum environments;
- Origin of the raw materials used by past societies;
- Unknown influence of past production methods on the environment;
- Phylogenetic information buried in microfossils.

Because of their chemical, structural and morphological complexity, many ancient and historical materials are yet to be understood at a micrometre level. Yet, molecular and supramolecular levels provide the ground for key processes occurring at this length scale. For example, a large part of the information sought is embedded within the composite material "imperfections": micro- and nano-inclusions, interfaces, grain boundaries, dislocations, texture effects, etc. Phenomena at the nanoscale could well play an essential role in corrosion, adhesion, mechanical behaviour of ancient and historical materials. In particular, the length scale between a few tens of nanometres and a few microns is especially important.

Depending on the nature of the object under study, the removal of a sample may be freely permitted, or forbidden (except, perhaps, in very limited amounts). In the former case, common objectives are: (i) to understand the heterogeneity at successive length scales, (ii) to study a statistically representative number of samples (or corpus) to reach relevant conclusions. In the latter case, adequate non-invasive methods are compulsory. Information at the nanometre level is today either collected through imaging at this resolution (scanning techniques, full field techniques, etc.) or through methods using a lower resolution (such as x-ray and neutron diffraction, small angle x-ray and neutron scattering, etc.) which provide statistical nano-information.

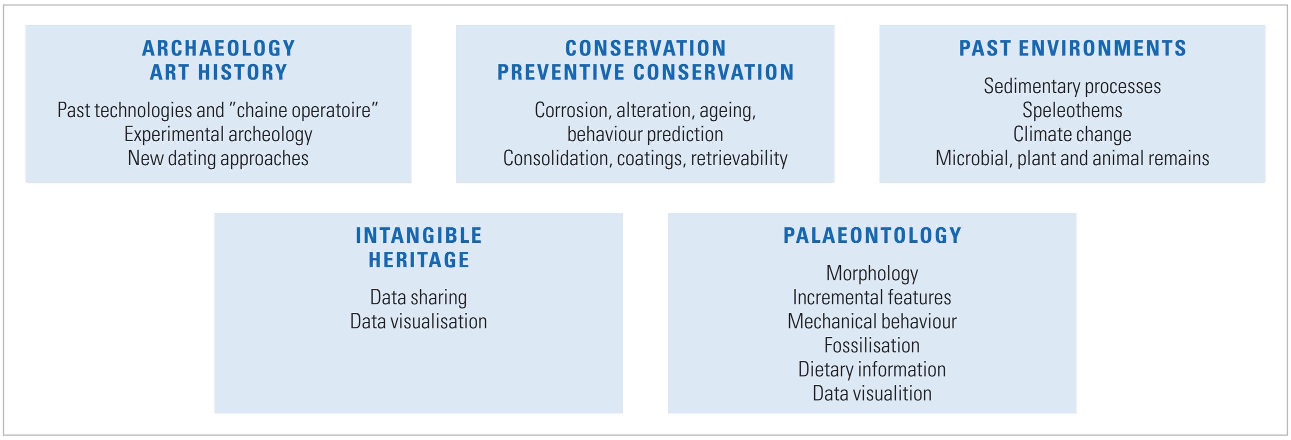

Fig. 5.11.1: Main fields of application of nanotechnologies for ancient and historical systems.

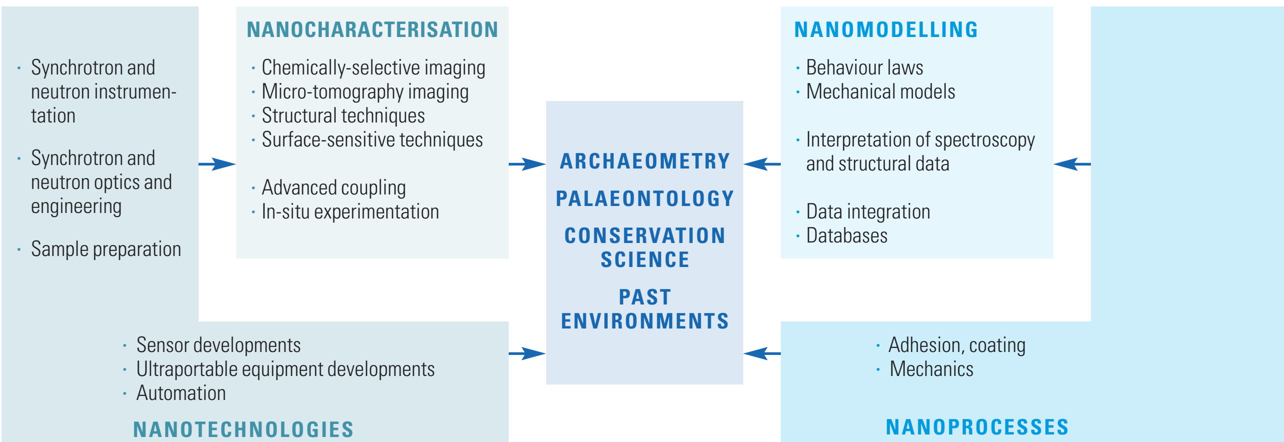

Fig. 5.11.2: Nanocharacterisation supported by nanotechnologies and nanomodelling through the understanding of nanoprocesses, towards a deeper understanding of ancient and historical systems.

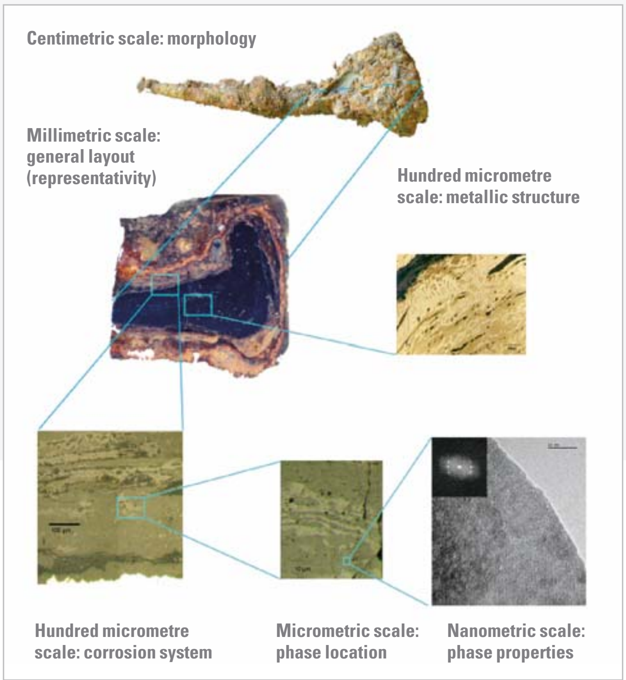

Fig. 5.11.3: In order to look at the corrosion of ancient archaeological artefacts as well as other ancient and historical materials: it is a necessity to apprehend an intrinsic heterogeneity from milli- to nanometre.

Overview of challenges in archaeometry

In the past years, archaeological research at the nanoscale has primarily been carried out on ancient technologies (nanoparticles in coloured glass and lustre ceramic decoration, ancient metallurgy, in-depth study of ceramic slips).

In years to come, major evolutions toward the nanoscale are expected in the following areas:

- Study of technological levels and ways of life of past societies through the examination of archaeological artefacts (such as ancient ceramic, glass or metals) found in well-defined contexts to suggest and consolidate manufacturing hypotheses;
- "Experimental archaeology" to reproduce past technologies and clarify the "chaîne opératoire" (sequence of production steps) used to make artefacts, including time-resolved study of crystal nucleation / growth, diffusion, phase transitions, adhesion, etc.;
- Degradation and aging mechanisms of archaeological artefacts, and the development of new conservation / restoration processes, means and measures (see also the "challenges in conservation science" part) with a specific focus on surface-sensitive techniques;
- Prediction of the long-term behaviour of material and of analogue/ model material alteration, to foster the development of resistant novel materials and the in-depth studies of long-term stable compounds (pigments, fibres, alloys, glasses);
- Support for the development of new dating approaches through a more efficient coupling of dating techniques and micro-analysis at large-scale facilities.

In archaeometry, synchrotron radiation and neutrons will be needed to collect:

- High-resolution chemically-selective maps for a clearer identification of the chemical compounds (crystalline and amorphous), particularly in object stratigraphies;
- Structural information from the identification of mineral phases to texture, grain size, etc. related to specific manufacturing technologies and corrosion mechanisms;
- Investigation of nanoclusters, nanocolloids and nanoparticles;
- In-depth interaction should be fostered with complementary large-scale infrastructures (laser, ion beam accelerators, dating facilities, etc.).

Overview of challenges in palaeontology, archaeo-zoology and anthropology

In palaeontology, a clearer understanding of the morphology of specimen at a smaller scale has been achieved in the past years. Study of insects, teeth, seeds, embryos at a micrometric and sub-micrometric scale have strongly benefited from the development of x-ray micro- and submicrocomputed tomography experiments at 3rd generation synchrotron facilities. Today, submicro- to nano-observations are already a reality used by palaeontologists at several synchrotron facilities.

The development of additional 2-D and 3-D chemically specific microscopy tolls is also foreseen to be of major interest for these fields of research.

In the years to come, the following major developments in nanoscale analysis can be extrapolated from existing research:

- Morphology of micro-organisms and nano-organisms for systematic palaeontology in complement to microscopy techniques;
- Local morphology of larger specimens in connection to complementary 3-D imaging approaches (laboratory and synchrotron-based µCT, surface scanning, MRI, etc.), including the morphology of fossil soft tissues;
- High-resolution observation of specimens embedded within amber or sediment;
- Mechanical, physicochemical behaviour, and alteration of biomaterials, including bones, feathers, teeth, hairs and soft tissues;
- High-resolution observation and analysis of incremental features and understanding of underlying mechanisms (e.g. incremental features in teeth, Sharpey's fibres indicating muscular insertions on fossil bones, etc.) for Evo-Devo models at a submicronic scale;
- Palaeobotany through virtual histological cross-sections;
- Biomineralisation and post-mortem fossilisation processes, with specific developments on the understanding of early diagenetic processes in complex environments;
- Retrieval of dietary and environment-related information. Imaging of markers providing information on animal domestication, on pastoral practices;
- Long-term preservation of biomolecules (keratin, other proteins, ancient DNA).

For these fields, synchrotron radiation, and to a lower extent, neutrons, will be needed to collect:

- Nano- and microscale 3-D tomography and related techniques to study high-resolution morphological features of small specimens and local observation of larger specimens;
- Chemically-selective mapping at high-resolution and structural information regarding fossil histology, mineralisation processes and dietary information;
- Coupling of macro-, micro- and nano- 3-D information among specimens.

The use of neutron techniques is usually limited due to the activation (related to U-series elements and REE).

Overview of challenges in conservation science

Our cultural heritage defines what we are, and is a source of inspiration which underpins current artistic and scientific endeavours. It also provides huge revenues, contributing in excess of €500bn to EU GDP through heritage tourism. Nanotechnology has been part of our heritage for over 1000 years. The earliest known nanometallic layers were produced in 9th Century Iraq in the glaze of lustreware ceramics.

In the modern field of cultural heritage conservation and research, there exists a huge potential for the application of nanotechnology in two areas: the use of nano-instrumentation and devices in chemical and physical analysis, and the application of the products of nanotechnology to restoration and conservation. Parallel with the development of materials and methods in these areas must come the application of advanced analytical techniques capable of monitoring processes on the macro- to nano scales, and obtaining spatially resolved and time-dependent information on, for example, the success of a protection strategy. Techniques capable of observing a process occurring in a controlled environment (in a gas, in a liquid) will also continue to be important.

Major developments in nanoscience can be predicted from the following areas:

- Nanoparticle-based conservation treatments, such as for the consolidation and protection of wall-paintings, the removal of sulphur and other aggressive agents (e.g. acids from wood and paper);
- Bonding of nanoparticles or nanostructures: nanomagnetic gels for artworks consolidation that can be removed magnetically;
- Engineering of nanoparticle ensembles that can at different times act as variable light filters, cleaning agents, sensors with control over functionality at the molecular level and so on, all the way up to larger groupings which may properly be regarded as nanobots;
- Use of mono- and multi-layers for the production of protective coatings (corrosion inhibition, protection from water vapour) for the protection of glass, metal artefacts;
- Composite materials that are light-weight and extremely rigid, or highly flexible, or elastic or which have properties such as high transparency combined with optical filtering etc. and which depend for many of their characteristics on nanofibres and nanoparticles, will find applications in the repair, support, and protection of heritage artefacts. A key acceptance criterion will be the absence of long-term damage to the artefact due to chemicals emitted from the materials as they degrade.
- Local investigation of artworks manufacturing techniques, based on high-resolution imaging.

For conservation science, synchrotron radiation and neutrons will be needed to perform:

- Chemically-selective mapping at high-resolution of chemical compounds (both crystalline and amorphous), particularly in stratigraphies;
- Investigation of structural information from the identification of mineral phases to texture, grain size, etc. related to specific manufacturing technologies and alteration features;
- Investigation of nanoclusters, nanocolloids, nanoparticles and nanolayers involved either in art techniques or protective treatments;
- Coupled micro- and nanoscale investigations;
- In-situ real-time investigation of accelerated ageing and alteration mechanisms and of the effect of chemical, electro-chemical, etc. conservation treatments and environmental conditions;
- Micro- to nano- 3-D imaging through tomography investigation of heritage materials (pore-size distribution, pore shapes continuity and dimensionality) and of the effect of consolidation treatments of glass, stone, wood, and other porous media, including time-resolved measurements;
- Additionally, nanotechnologies are of key relevance for intangible heritage, when one of the major aims is the digitalisation and long-term storage of very large quantities of data.

Following a century when the over-optimistic application of new materials and techniques to unique artefacts and artworks lead to numerous disasters (e.g. irreversible damaging of wall paintings by soluble polymer "protective" coatings, time-delayed bleaching of pigments in major artworks through the application of insufficiently tested analytical techniques), a strict ethical framework for the scientific

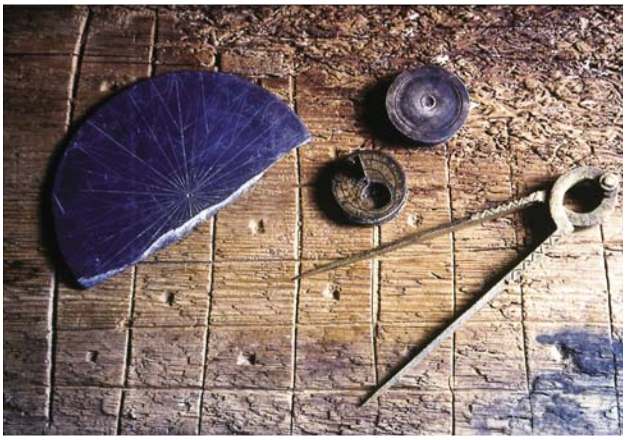

Fig. 5.11.4: Wood, stone and metal from Henry VIII's flagship "The Mary Rose". Can nanotechnology help conserve these artefacts?

study and conservation of heritage artefacts has evolved and is documented in various charters such as the Venice Charter (1964). The underlying principles of these include reversibility (treatment must be reversible), retreatibility (present treatment must not interfere with future treatment), compatibility (treatment must not have negative consequences and must also be aesthetically acceptable) and minimum intervention (do as little as is necessary).

The implication of new methods of conservation based on nanotechnology is profound: the acceptability of a method must be based on rigorous testing over several years, and not on the prevailing scientific fashion; a treatment which is suitable for a modern material which will be discarded after a few years of use may be wholly unsuitable in a heritage context. Nevertheless, when faced with the total loss of an artefact, nanotechnology may offer the safest route for its survival.
Overview of challenges in past environments studies

A variety of substrates can provide information on past climatic conditions. In particular, systems such as layered sediment (continental and marine), ice cores and speleothems have provided detailed recording of climatic variations and the environmental response to these changes. On systems where the layering is not too much perturbed during deposition and further recrystallisation, sub-annual resolution has already been obtained using synchrotron x-ray fluorescence and provided accurate climatic information.

In the years to come, major evolutions toward the nanoscale are expected in the following areas:

- Study of the climatic records;
- Understanding of deposition processes;
- Complementary analysis to dating.

To study past environments, synchrotron radiation and neutrons will be needed to perform:

- Chemically-selective mapping at high-resolution of chemical compounds (both crystalline and amorphous), in stratigraphic records;
- Structural information from the identification of mineral phases to texture, grain size, etc.;
- Investigation of nanoscale phase transition occurring during deposition and diagenesis processes;
- Investigation of microbial, plant and animal remains within sedimentary records using on-development x-ray microscopy techniques.

Role of synchrotron radiation and neutrons sources

Key features of synchrotron radiation and neutron sources for these fields will be to provide:

- Joint characterisation at the micro- and nanoscales;
- Adapted support to the user communities;
- Strong interaction with other types of large-scale facilities.

Key instrumental and methodological improvements should be sought for in the following areas:

- Development of high-resolution imaging x-ray techniques (fluorescence, absorption, diffraction, small-angle scattering) for coupled 2-D characterisations;
- Tunability between microscale and nanoscale characterisations. It has indeed to be noted that state-of-the-art imaging techniques whether in scanning mode or in full field mode provide at best megapixel fields of view. It is therefore today hardly possible to interconnect data acquired at micro and nanoscale.
- Development of 3-D x-ray tomography techniques, 3-D confocal imaging, including in chemically-selective 3-D modalities;
- Development of techniques providing nano-information at a lower resolution (SAXS/SANS and WAXS), as well as "white beam" XRD at true nanoresolution, surface scattering and grazing incidence techniques;
- Advanced coupling of characterisation methods at the large-scale facility beam lines, providing information on organic/inorganic, amorphous/organised fractions, etc.

Complementarily, additional developed equipment and data collection modalities should be optimised to foster:

- In-situ measurements under monitored environmental conditions (corrosion cells, temperature and relative humidity controls, etc.);
- Data integration between microscale and nanoscale characterisations.

To allow such breakthroughs, new instrumental developments are a prerequisite, some of which will also require inputs from nanotechnologies (partly to be developed at large-scale facilities or associated "foundries"):

- Nanofocusing optics (including high-resolution Fresnel zone plates), and more generally optical elements able to provide stable and reliable observations at the nanometre level. This includes not only the development of new devices but also their fabrication, as some of these optical elements are indeed consumables. Their low availability is already a limiting factor for the development of nanotechniques.
- Set-ups for nanocharacterisation involving nanodisplacement of samples and mechanical control and stabilisation (piezo-, feedback, etc.);
- Nanolocalisation and nanomarking of the samples in order to precisely record the studied areas and relate it to observations at a larger length scale;
- Low noise detection chain due to the low analysis and/or sampling volumes;
- Development of new instrumentation using nanotechnologies: ultraportable and laboratory characterisation equipments, digitalisation, data storage, visualisation, etc.

Coupling with other large-scale facilities at the European level

Due to the high level of cross-disciplinarity required for these areas of research, dedicated support are already asked for at large-scale facilities, as illustrated by the FP7 project CHARISMA, which combines synchrotron, neutron and ion beam analysis techniques for conservation sciences.

Developments at the nanoscale will require even tighter integration and stronger user support. In particular, pre-experimental and post-experimental requirements will constitute key steps to foster a fast, in-depth and efficient implementation of the new nanodevelopments for these fields of research. This includes:

- Sample preparation procedures that may be particularly difficult for the heterogeneous ancient materials, though of key importance for nano-focused imaging;
- On-demand specific support to experimental proposal preparation, awareness of the community;
- Development of analytical standards and reference materials;
- Data processing, particularly for 3-D and quantitative 2-D compared to point examinations;
- Modelling of material behaviour at the nanoscale for mineralisation, alteration, conservation, etc.;
- Dissemination to researchers, end-users (archaeologists, curators, etc.) and industry;
- Ethical considerations, primarily regarding conservation measures, that should be researched as part of these developments.

Conclusions

- 2-D and 3-D imaging techniques (including chemically-sensitive modalities) are of key relevance regarding archaeometry, palaeontology, conservation sciences and the study of past environments.
- A clever coupling of macro-, micro- and nanocharacterisations are an absolute pre-requisite to the in-depth study of ancient and historical materials. They could first develop as pilot studies, then at a major scale provided adequate instrumentation and support are put in place. Synchrotron and neutron facilities offer the unique opportunity to combine macro- and nanocharacterisation and could therefore allow efficient characterisation and integration of information at the successive length scales.

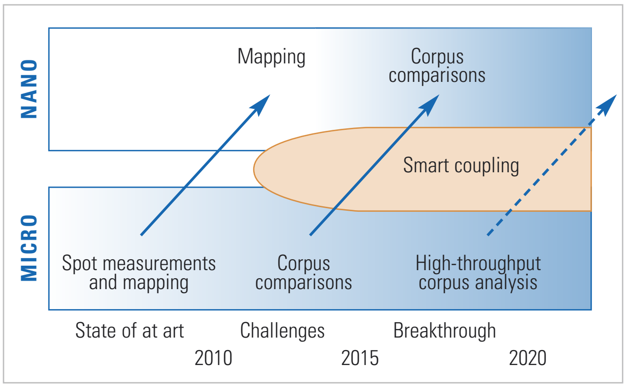

Fig. 5.11.5: Roadmap for ancient and historical systems.

- Dedicated support at the interface between LSFs and the user communities, both regarding basic and applied research is required, as currently developed for other areas of research such as life sciences.
- The availability of beam time and adequate selection procedures is a crucial parameter for the study of corpuses of samples in connection to the expected high variability of ancient and historical materials at the nanoscale.

5.12. SECURITY AND SAFETY

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The various applications of nanomaterials in security and safety are strong candidates to become "key" for the long-term penetration and commercial usages of nanotechnology. In several cases, environmental protection application can be considered as part of safety and security, in particular when issues such as disasters related to natural and man-made environment are concerned. Security technologies also have to face the ethical compromise between security benefits for human beings and citizen liberty reduction risks. Both of these aspects are already integrated in nanotechnological research. An example of this contradictory assessment is given by the fact that security technologies are foreseen as being small, diffused, ubiquitous and pervasive, but to some extent they also have to be used in smaller quantities in the right places and at the right time; here, one refer to the concept of vectorisation in nanomedecine.

Fig. 5.12.1 summarises the perimeter of the global security domain, including the CBRN/E (chemical, biological, radiological, nuclear/explosive) threats.

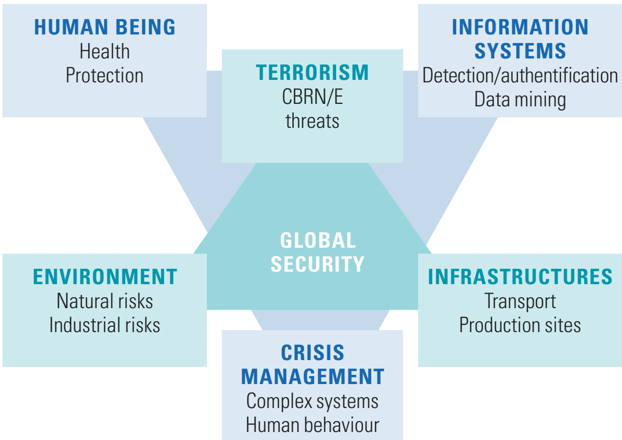

Fig. 5.12.1: Security/safety in key technologies.

Scope

Nanosafety/nanosecurity around the human being (terrorism, murder, violence):

- Malicious attacks of human beings against the human being, and could include multi-threats or the use of weapons of mass destruction (WMD). It deals with prevention, protection, operational risks for professionals, decontamination and prophylaxes;
- Protection through unplanned, accidental risks of the person, directly concerned with the person. All along the "crisis chain": professionals who intervene in the core area of accident, those in the second areas where extra contamination has to be avoided and where first aid is brought to victims (individual, collective) as well as to citizens;
- Security in the supply chain, being in the midway between security and safety, e.g. illicit copy of objects that can hurt both incidentally or voluntarily persons and societies (illicit copies of medication and of hardware);

Security and safety of critical installations can have a dramatic impact on the way of living. This implies the security of the installations themselves like power plants, chemical, petroleum installations, transports installation and, in future, blackouts of the communication systems, but also their consequences and moreover their interdependencies with other infrastructure (see 2003 Northeast Blackout).

Environment can improve or decrease the quality of life: it is a factor indirectly linked to safety in two ways:

- Influence on the health/integrity of the person;
- Influence of the natural or man-made risks for humans.

Nature of nanotechnologies for safety and security

Nanotechnology can lever safety and security through several routes, falling in two overall categories:

- New nanotools and methodologies
  - Identification of **new tools for structuring material** at the nanoscopic level, for instance in order to place molecules or create nanosensors (e.g. nanoparticle-based biosensors for the detection of biomarkers/biodiagnostic) or nanostaining for molecular and in-vivo imaging.
  - Creation of **new ways to assemble and functionalise** matter at a nanoscopic level. Such materials will become "smart" by an adequate association of "intrinsic" properties and "added" properties (for instance for selective absorption – e.g. nose – or news ways of in-vivo drug delivery by small scale systems, for example with biodegradable long circulating polymer nanospheres, delivery of molecules e.g. counterfeit applications).
  - Tools for interfacing the nanoworld to the macroworld. This can include very simple tools such as handheld optical microscopes (obviously engineered adequately), and software tools for "reading" specific, well-targeted properties of the nanoworld. Counterfeit is one of the fields where such technologies are well-suited.

- New nanomaterials
  - Creation of **new materials with new properties** based upon their nanoscopic structure, to meet the contradictory demands of security (robustness, sensitivity, versatility, selectivity). By utilising physics, functionalities, and design strategies that are different from regular photonics, one can think of producing tiny waveguides, microscopes on a single chip, better optical communications equipment, and new chemical and biological sensors. Material should also be seen as biological material and include novel biomaterials through molecular self-assembly for the restoration of tissue alterations, new generation of chemical agents and so forth.
  - Combining the ability to **manipulate molecular structures with advances in genomics** and proteomics and other biological sciences will create a wealth of new research opportunities. By putting these unique properties to work, scientists are developing highly beneficial dual-use products in medicine, electronics,

and many other industries that will also provide enormous defense and homeland security capabilities.

- Engineering of new devices that **can couple or merge different technologies (physics, chemistry and biology), into a single sensor**, taking into account the benefit of each technology, their ability to communicate with each other (at the local stage), their self-poweredness, and adding smartness by an adaptative and powerful signal processing such as data fusion: this trend is often called "system of systems" and is related to the "smart dust" concept. In this concept, the design of biochips combining nanominiaturisation (nanofluidics) and optical nanodevices allowing dynamical measurements for proteomic or genomic purposes are now revolutionising detection (including for high throughput screening of therapeutic compounds) or diagnosis by allowing for more rapid and more convenient highly multiplexed detection.

Importance of nanodevices for safety and security (Fig. 5.12.2)
The importance of nanodevices can be paramount for the segments which are discussed above because of:

- Reduced volume, implying large-scale deployment without being noticed by the malicious organisation and person, or by the persons that are protected;
- Robustness to be used in every situation and to be implemented by people who do not have a specific nanotechnology knowledge;
- Reliability to provide a repetitive significant answer for a given threat;
- Sensitivity: ideally for many threats, the detection of the first molecule/particle/pathogen is crucial in case of a crisis so that the nature of the alarm can be determined as soon as possible, so that prevention/protection means can be deployed efficiently;
- Selectivity is of prime importance in the concept of "false alarm" in addition to sensitivity, or for devices that could capture toxic substances and avoid extra-contamination;
- Versatility seems to be contradictory with the two above-mentioned characteristics once a wide range of sensitivities should compromise with high selectivity, but these functions can be achieved by nanodevices that could decide themselves to adapt/re-configure their properties (first wide band, then narrow band analysis). All these performances go under a meta umbrella called ROC: Receiver Operating Characteristics;
- Rapidity of detection: in crisis situation involving human lives, rapidity is the key factor that governs the response/treatment and minimises impact;
- Rapidity and readiness of implementation: large-scale deployment which seems often necessary for efficient prevention. In fact such deployment is specific to the protection aspect, and therefore key to both security and safety, perhaps much more than in other domains.

Convergence and its importance for safety and security
The security/safety applications will benefit from the multiple convergences that underline the enabling nature of nanotechnologies.

Convergence between top-down and the bottom-up approach. The continuous downscaling of traditional microelectronics technology is extremely important for safety and security, since it adds additional dimensions in the traditional "processing" and "communicating"

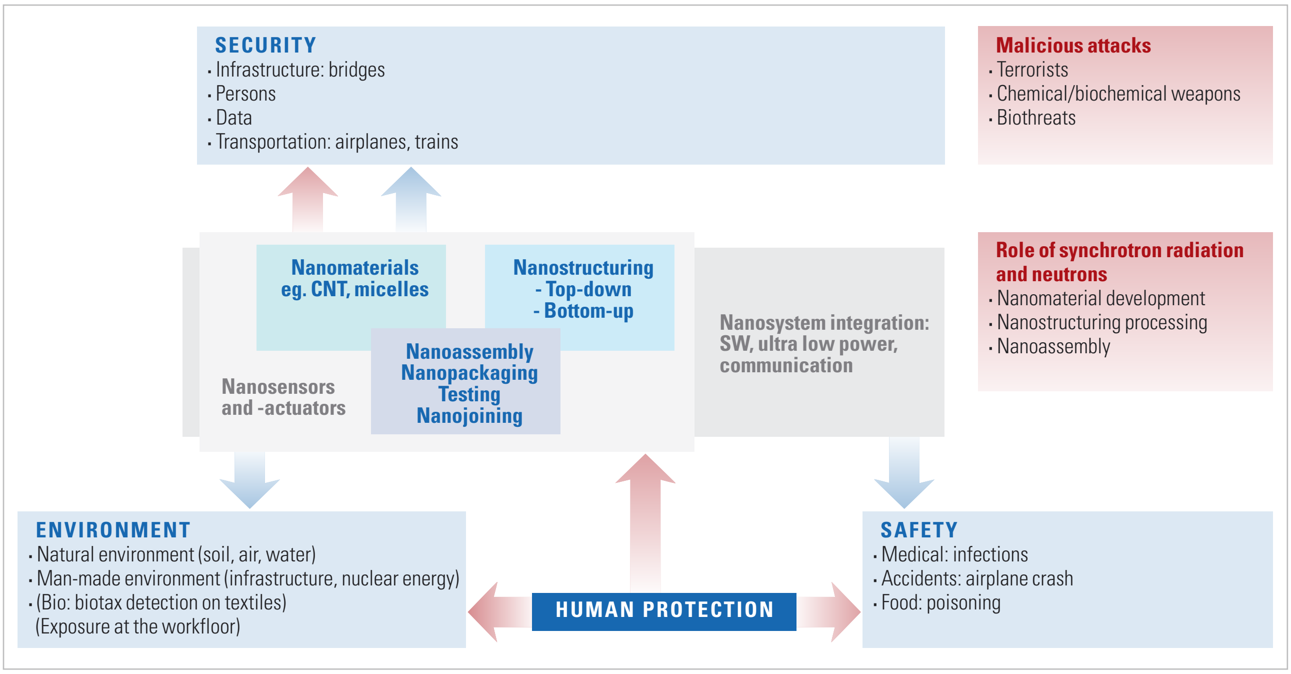

Fig. 5.12.2: Nanomonitoring for the safety, security and environmental protection of the human being.

capabilities of integrated circuits. The new dimensions include "sensing", "actuating", "powering" and "interfacing". Safety and security cannot exist without such new functions. Their implementation at the nanolevel allows the very existence of new functions.

The bottom-up structuring of matter at the nanoscale level further reinforces the arsenal of technological means available for the aforementioned additional functions: for instance, self-organised matter can provide new, unforeseen functions, or realisation of previously existing functions at a dramatically decreased cost, allowing large-scale implementation, which is critical for safety and security functions.

Then it is clear that the first dimension of convergence between top-down and bottom-up approaches, depicted in Fig. 5.12.3, can be critical.

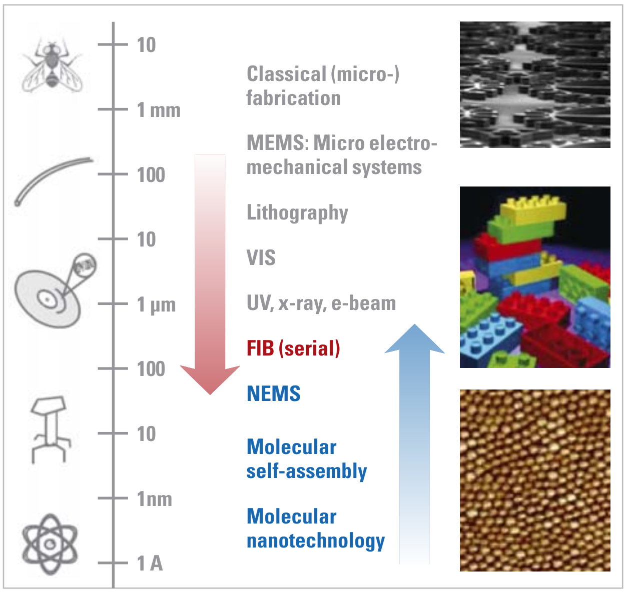

Fig. 5.12.3: The convergence between self-assembled nanoworld to microsystems that act as bridge tools between the nanoworld and the macroworld.

The convergence between nano-, bio-, information and cognition technologies (NBIC) contributes to the further reinforcement of the techniques available. Such enrichment is very important because the applications field is highly fragmented between a lage variety of security and a large variety of safety applications. Biotechnology: especially for CBRN/E (chemical, biological, radiological, nuclear and explosive), threats will benefit from the merging of both nanoscience disciplines (hard and soft matter) and biology. For instance, the use of specific antibodies onto nanodevices opens new ways for multiplex detection of chemical, biological or explosive agents; The time evolution of the nano- to bio-convergence is depicted in Fig. 5.12.4, which also gives an illustration of how we move from the molecule level (chemistry) to classical biological agents, which in turn are improved and at the end are foreseen to be encapsulated in ad-hoc nanostructures.

- Information because as soon as a threat is known, people and systems can react, afterwards it is a problem of implementation in a crisis environment. Communication capabilities should also be seen directly at the nanoscale;
- Cognition and especially "crowd cognition" or "crisis behaviour cognition";
- Energy aspects: autonomy is a key factor in the concept of large diffusion threats, autonomy has to be designed at the nanoscale where energy losses and efficient use of energy can be achieved at a higher level than at the macroscale.

We identify in the development of nanomaterials for security the following overall trend: structuring of both top-down and bottom-up technologies in a multi-disciplinary environment with ad-hoc intelligence.

Criteria for future security – safety – environment research

Security research has to take into account the following aspects in the chain for future security-safety-reliability research:

- Nanomaterials for advanced sensor and actor nodes and systems;
- Self-organised security chains, "system of systems concept" etc.;
- Nanomaterials testing methods (combined safety, reliability and security properties);
- Nanomaterials diagnostics (extremely small quantities, many substances including bio-pathogens or bio-inspired chemical agents;
- Monitoring of nanomaterials properties ("complex "analysis), e.g. long term-monitoring;
- Monitoring from very small to very large areas;
- Safety and reliability aspects of nanomaterials research;
- **Clean-tech aspects** of nanomaterials and nanotechnology for nanosecurity applications, their innocuity for long-term life cycle, their degradability or "re-usability";
- **Combined social as well as technical aspects** of security (and safety, and reliability);
- Risk analysis and risk management based on advanced nanomaterials knowledge.

Specific trends include:

- **Micro-/nano-integrated sensors:** The actual microdevices start to be technically feasible and plausible enough to be used in field applications: the nanosensors and actuators development are as follows:
  - Chemical sensing devices, using nanosensors as new developments for lead detection (meaning safety applications, for instance for exposed workers). Nanotechnology and biotechnology converging at fast pace is seen as the plausible solution for providing e-nose devices with enough sensitivity to compete with the dog nose;
  - Nanogrooves and protein nanoarrays: Development of receptacles for optical indicators following the concept of protein nanoarrays which have nanoreceptors, engineered according to the detection techniques;
  - Soft (bio-) to hard (electronic) nanostructured material attachment, biochips, optics, quantum dots, quantum wires, sol-gel,

thin films deposition, fluorescence, absorption technics, microbalances, chromatic sensors, etc.;

- Self-assembled gratings for nanodetectors used for chemical detection on large surfaces – walls, textiles, polymers. Mechanical detection at the atomic level using atomic probe arrays ;
- Novel nano-actuating mechanisms, providing the action towards the threat. Multiple types of nano-actuation mechanisms are in development depending on the threat or hazard to be mitigated. This can be a bioreaction based on nanoparticles or nanostructures; on a more macrolevel it can also be nanotechnology-based components for miniaturised devices i.e. nanoscale rotor where two opposite charged nanopaddles activate a rotor.

- **Nano-biotechnologies** should play an important role in the response to a CBRN/E multi-threat. For the full understanding of the mechanisms of toxins at three levels it is necessary to identify menaces and propose diagnostics, therapeutics and prophylaxis:
  - At the genomic scale: for example, understanding gene expression profiles through different means such as mRNA profiling, is of major importance to detect a disease, identify the corresponding pathogen and its way to change metabolism and then find new diagnostics and therapy to fight against;
  - At the protein scale, huge work still remains to be done in order to better identify and characterise the protein's world and their implication in some major pathologies of the B threat, in order to design new therapeutic targets.
  - At the integrated scale: this is certainly the main challenge that nano-biosecurity will have to face in the coming years. In addition to fully integrated nanodevices (as mentioned above), the use of non-invasive characterisation techniques (NMR, IMR, Spectro- NMR, new trends in High Resolution NMR and molecular imaging) would allow to complete the chain to understand how such systems interact in a complex living system and to design novel therapies and medical protocols.

- **Protection technologies:** professionals who would be the first humans in the area of a terrorism attack for instance have to be protected.
  - The protection should be basically "adaptable" once time has elapsed after the attack, the level of information increases (often information that is acquired by embedded sensors worn by these first actors); the level of protection should be increased and adapted to the event. This implies communication but also the ability to reconfigure the properties of the protection suits and the second area protection devices.
  - For safety, the material aspects become predominant. Nanomaterials/technology is key to improving security-related engineering properties, i.e. structural strength (nanocomposites) from light indoor structures to large structures such as airplanes or civil engineering works. Performance resistance that can be related to security matters cover aspects such as improved friction and thermal conductivity or isolation capability (aerogels),

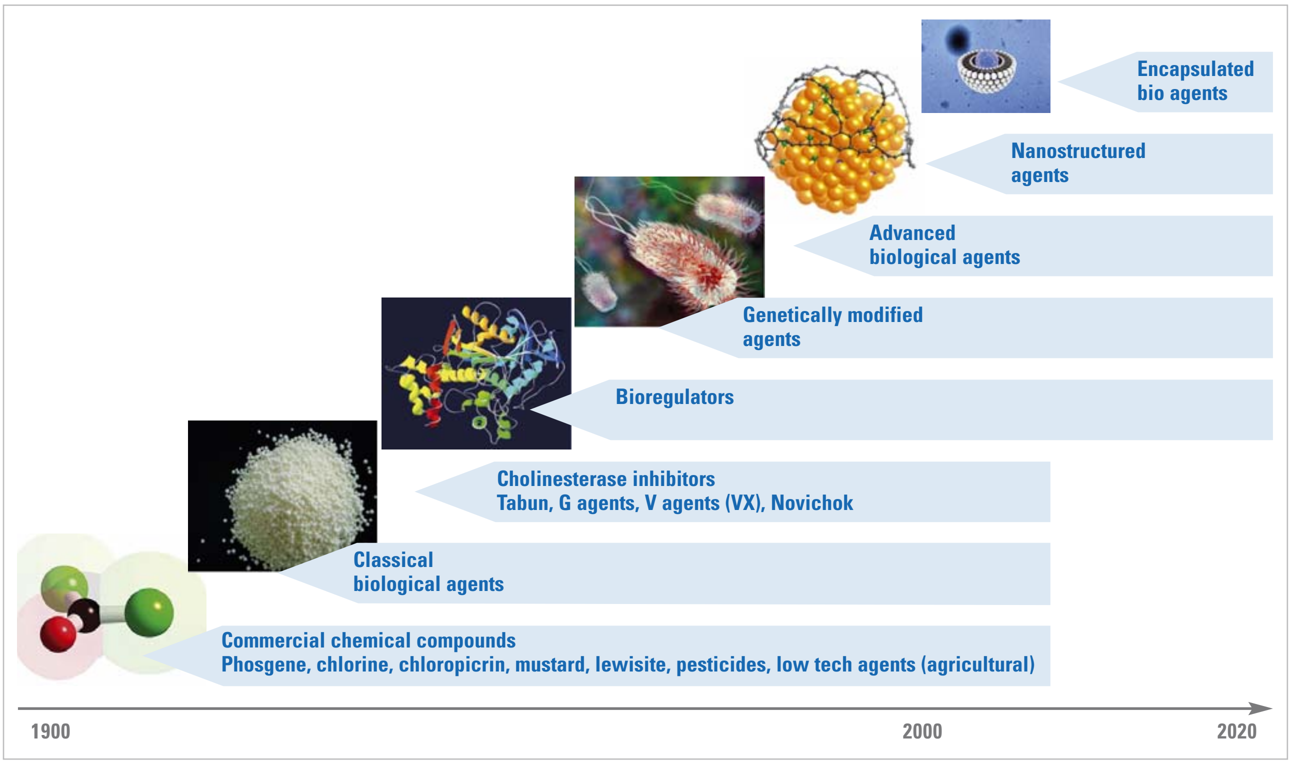

Fig. 5.12.4: Roadmap for bio-nano agents.

mastering of conductivity (nickel nanofilaments or multi-wall nanotubes), improved resistance to wear as well as optical properties and hydrophyilicity or hydrophobicity. Control of release of chemicals – through micelles – can be a tool to control properties over time, in particular for structural improvement applications. Fig. 5.12.2 gives an overview of the potentials for nanomaterials research and development in security, safety and environment.

- **Decontamination/remediation technologies** will also play a major role in crisis management: aerogel with nanodesign cages (cyclodextrines ou mesoporous sensors) can be used to capture toxins so that one can avoid extra contamination and later make it easier to clean the areas by removing this "smart" film from its location or from victims. Here again the "intelligence" of the nanofilm relies on its ability to sort/filter substances so that toxins are stopped but air can pass through for respiration for instance.

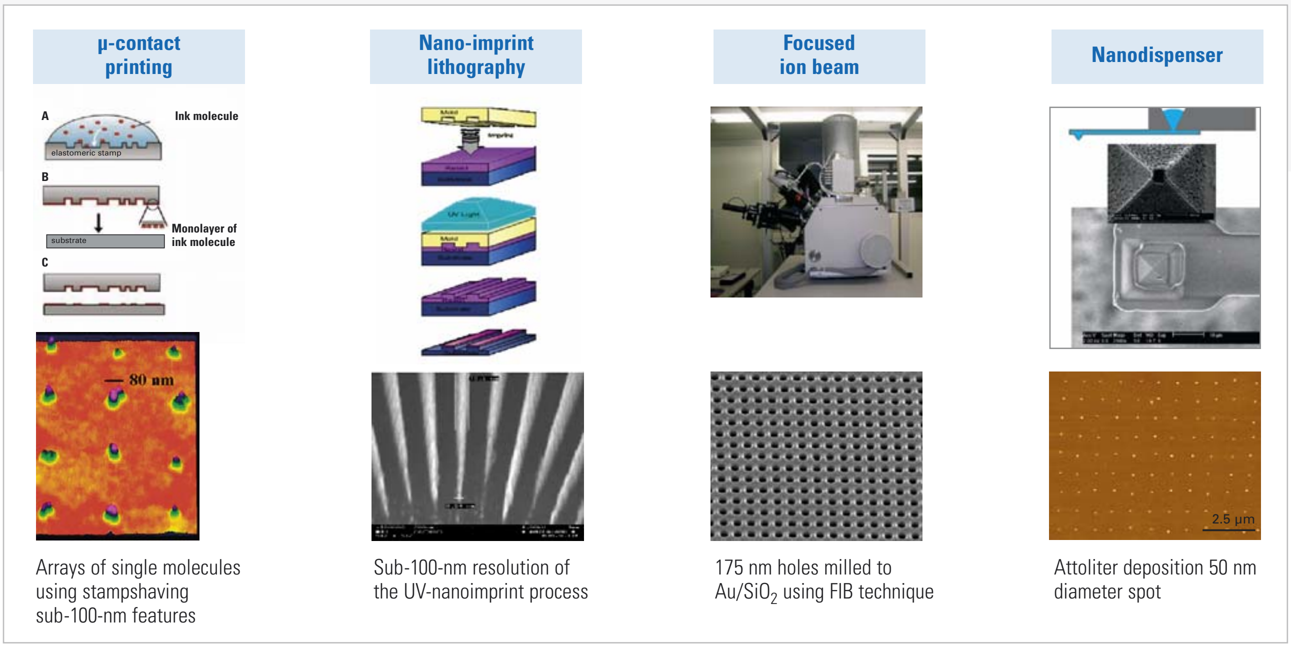

Fig. 5.12.5: Top-down technologies for nanostructuring.

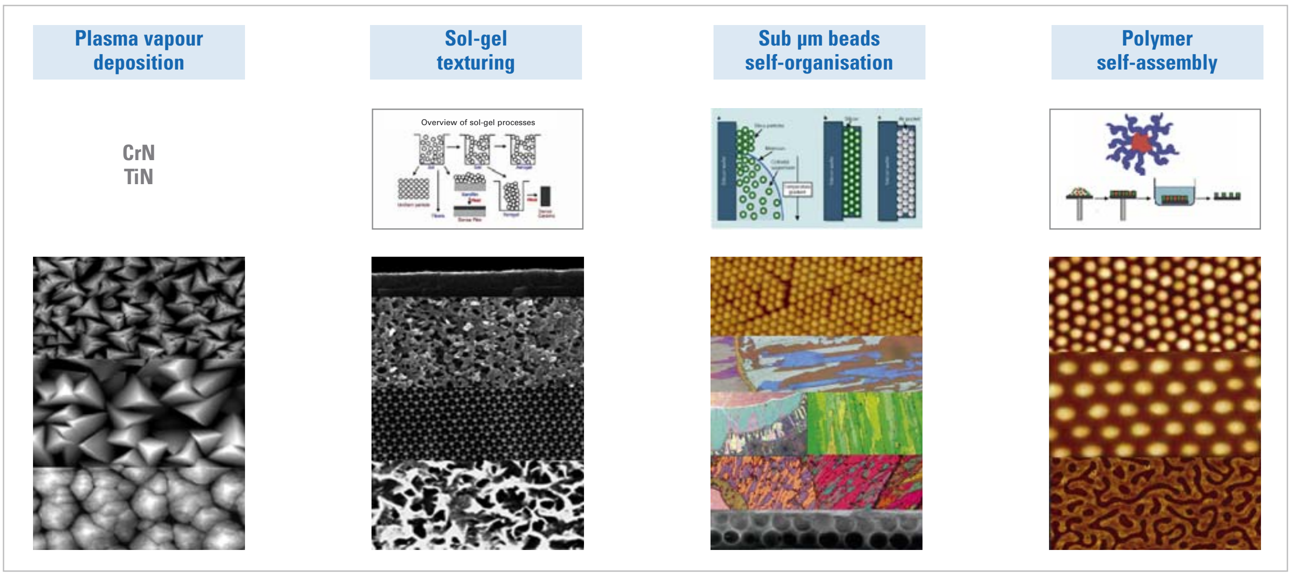

Fig. 5.12.6: Bottom-up technologies for nanostructuring.

- **Implementation and communication technologies:** Extremely interesting challenges beyond the nanoworld are emerging here: The virtually "invisible" nature of the sensing devices means a very high number of devices, perhaps redundant in number.
  - Networking and common intelligence of individuals: Today some tenths of sensors can be networked, in the future, the networking of tens of thousands, the structure and possible the clustering has to managed;
  - Type of intelligence: it has to do with (conventional) electronic intelligence or with self-located, new types of intelligence based on the physicochemical properties of the devices (e.g. coordinated reactivity of a cluster of nanodevices);
  - Energy generation: even if the individual system requires a tiny amount of energy, the very high number of sensors can, by simple arithmetic, considerably increase the energy to be used and to be evacuated. New types of harvesting at the sub-micronic level will be key enablers for such technologies. This can be based upon the generation of energy by biological species (e.g. microbes) or by nanolevel scavenging;
  - Nano-actuation factor: intelligent actuators, as for instance surfaces that react to their chemical environment (eg. micelles) are certainly going to become a key factor in tomorrow's nanoworld.

Technological tools for nanotechnological devices, subsystems and systems

For developing nanosecurity and -safety technologies, a large variety of design techniques can be envisaged (Fig. 5.12.5, Fig. 5.12.6.).

Role of synchrotron radiation and neutrons (Fig. 5.12.7)

The European research infrastructure must play an important role in the design/synthesis/characterisation of specific nanomaterials for security, especially in solving the compromise between sensitivity and versatility (Fig. 5.12.5). The key areas of research include:

- General crystallography of functional structures (in particular sensors);
- Detailed understanding of biomolecule dynamics;
- In-vivo characterisation of functional nano-architectures;
- 3-D patterning and characterisation of functional arrays.

It is worthwhile to mention here that non-technical parameters, where nanotechnology could contribute will be important for the large-scale acceptation. These factors include:

- Dimensions and intrusiveness to the environments;
- Cost (both Capex and Opex);
- Environmental cost and danger;
- Flexibility of integrating everywhere in particular, with new, inacceptable up to now methods (cf. spraying);
- Perception of non-hazardous introduction by general public.

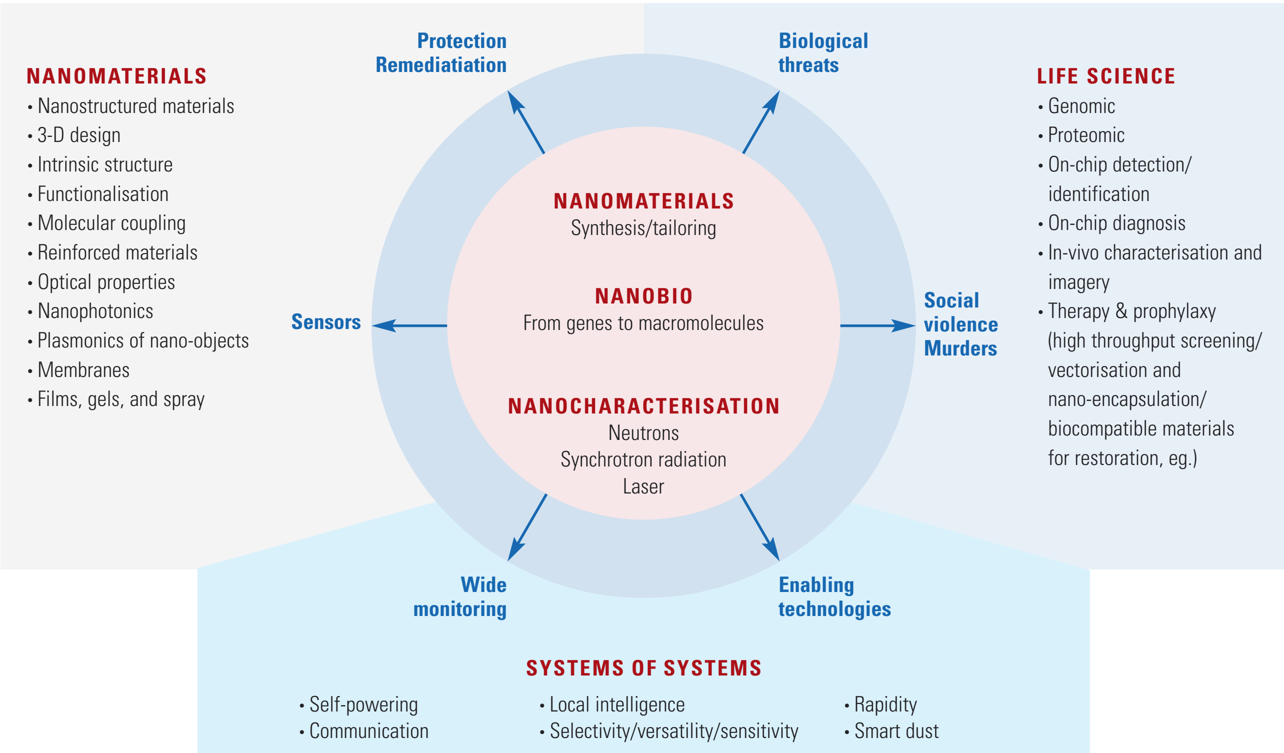

Fig. 5.12.7: Application wheel of synchrotron radiation and neutrons for security/safety.

	NANOENGINEERED CHEMICAL SENSORS		POWERING	COMMUNICATIONS		NEW SURFACE AND BULK PROPERTIES
SECURITY	(Bio-) Chemical	Physical	• New powering methods (microbes in-body) • Self-power management	RF or optical communications	Protocol @ Data fusion For high number of sensors	Large surface molecule attractors
	CNT	• Self-assembled 2-D/ 3-D periodic structures • Top-down engineered structures				
	Proteins					
	Soft (Bio-) on Hard (Si) coexistence and convergence					
SAFETY	Nanosecurity					Intelligent diagnostics
	Nanorobots					
ENVIRONMENTAL PROTECTION	Sensors for harsh environments, high robustness, high reliabiltiy					Mainly man-made structures • Aircrafts • Mechanical parts

Table 5.12.1: Security/safety in key technologies.

The combination of technical feasibility and the aforementioned non-technical matters, will contribute to the success of penetration of nanotechnologies in these key applications for the human being and for the changes to expected in our lives.

In future the "Security, Safety – Reliability – and Environment" research must be combined. These topics have always been research individually and there is an urgent need to set up interdisciplinary research programmes.

Perspectives

The emergence of nanotechnology concepts dedicated to safety and security applications is now a reality.

The endeavours towards industrialisation are multiple, in particular due to the fragmentation of the application fields, and the maturity of industrialisation asymmetric.

The efforts made in developing new sensors based on nanomaterials as carbon nanotubes are a first illustration. This research has been initiated at the end of the nineties and now multi-year programmes are under progress (e.g. works from Naval Research Laboratory in USA or CEA in Europe on the development of resistors or transistors with single-walled or multi-walled CNT for detection of chemical agents).

Another illustration of this research effort in nanotechnologies can be offered with the development of silicon nanowires for biological detection of pathogens agents (e.g. see works from CALTECH in USA or CEA in Europe).

All of these research programmes have a common link in the combination of nanotechnologies from electronics with surface functionalisation from materials science or biotechnologies. Presently, research is still on the laboratory scale in this domain.

Some of the most advanced programmes have now reached the component validation éeveé which means that proofs of concept have been successfully brought under the form of laboratory demonstrators giving significant performances in terms of detection (sensibility, specificity, selectivity). The less advanced programmes (or most recent) are in the feasibility phase.

In certain cases, however, in particularly in fields related to the security of documents and tracing of products (counterfeit), nanotechnology-based solutions are down to the marketplace today (e.g. solutions provided by the French Hologram Industries S.A.).

More sophisticated solutions, in the same field of security and counterfeit are close to commercialisation, as of today. In all cases when such maturity has been achieved two major factors have been decisive:

1. User-friendly tools for interfacing the nanodevice to the macroworld. User-friendliness is the most pressing requirement, since the hurdle, most probably to be faced, is the precise positioning of the nanostructure to be addressed in front of the reading equipment. As a futher requirement, limited volume, simplicity and facility of realisation of such tools is also important, in order to maintain economic competitiveness, as related to established techniques.

2. Adequate techniques for large-scale implementation which exploit the potential of large-scale production. Further elaborating, when this has to do with top-down manufacturing techniques, here the expected market volume has to be large in order to justify the economies of scale required by such techniques.

Nanoelectronics is typically a very large family of technologies that enters in the top-down category, and obviously today semiconductor industry, already producing devices with features of 65 nm and researching well below, is in the phase of exploiting scale economies, (albeit not only for security and safety, but with a more generic business target).

Interestingly enough, the association of the aforementioned nanoelectronics devices with nanosensors and nanoactuators is one of the most challenging topics that industry attempts presently to face. The European Industry driven Joint Undertaking ENIAC is a concrete effort towards this direction. An extension of this effort focusing principally on nanoelectronics, is the European EPOSS platform that targets initially the extensions of microelectronics to microsystems, with as a final objective the nanosystems.

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In conclusion, nanotechnologies for safety and security offer a real opportunity to identify scientific and technological breakthroughs. On the one hand, the limits of current technologies give real perspectives for nanotechnologies in the next decade. On the other hand, the success and the industrial penetration of applications will really be connected to the maturity of applications for mass market and their societal acceptance.

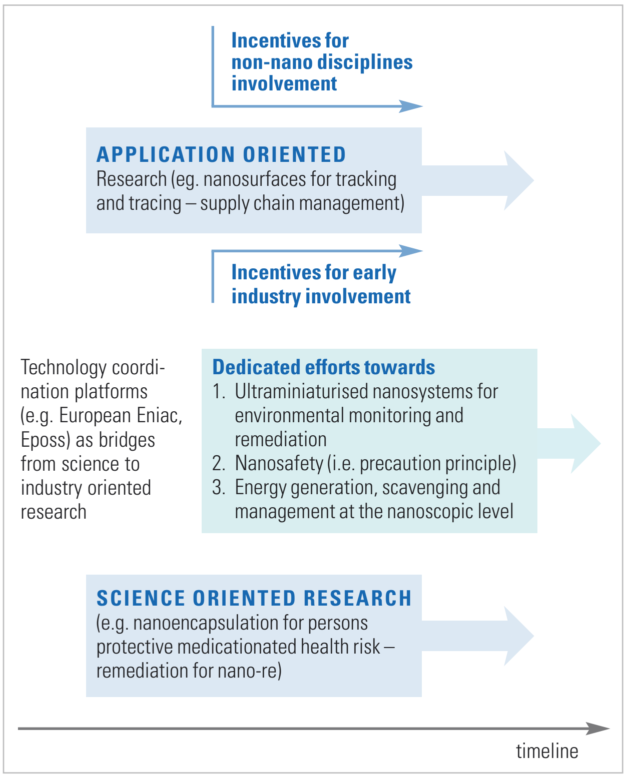

Fig. 5.12.8: Safety issues in nanomaterials.

The challenges faced require concurrent efforts and support by traditional, non-nanotechnology industry in a system approach. Mechatronics, optics, electronics and software are needed.

Early association of industry, through dedicated incentives for participation in the R&D efforts is a must in order to orientate resources towards needs. However, a parallel effort towards purely research needs to accompany such incentive to maintain long-term incentives.

The convergence of nano- with bio- as well as with electronics and cognitive, as well as the top-down/bottom-up approach call for coherent efforts and coordination to avoid duplication of efforts.

To optimally exploit the miniaturisation resulting from the nanotechnology energy sources at the same order of dimensions will be of particular importance during the years to follow. The diversity of applications will call for a diversity of energy sources; such fragmentation is already observed in energy scavenging techniques at the microlevel.

Safety related to the nanodevices and nanomaterials is also an upcoming societal need. The European Commission has initiated such efforts by financing under its NMP FP6 Research Programme an effort towards this direction with the NanoSafe project.

The aforementioned lines could be outlined in Fig. 5.12.8.

5.13. DIRECTIONS FOR NANOMATERIALS TECHNOLOGIES

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Over the next two to three decades, nanomaterials will have a substantial impact on many technologies ranging from electronics to medicine. The crucial point is that the properties change dramatically when the dimensions of the structure are in the nanoregime since quantum phenomena play a dominant role and the materials surface/interface becomes very important. We are just beginning to learn how nanosized materials “use” those mechanisms to “obtain” superior properties. Hence the forthcoming decades will be devoted to two main goals:

i) a fundamental understanding of the relevant physical processes; and
ii) the development of technologies enabling those properties to be exploited.

This section highlights the future research for the whole spectrum of technologies (see Fig. 5.13.1).

Nanomaterials developments will be key to advances in:

- Aerospace, e.g. self-monitoring and active aeroelastic flight surfaces, leading to more efficient flight surfaces, safer flight;
- Energy, e.g. nanocomposites using clays to increase specific stiffness for wind turbines thereby power generating capacity;
- Nanomachines, e.g. microjets able to control airflow over wing or engine surfaces;
- New materials, e.g. scratch resistant coatings, smart materials, sports goods, etc, opening up completely new commercial avenues.

Electronics and communications (Fig. 5.13.2)

Currently technologies i.e. nanoelectronics, nanophotonics etc rely on the down-scaling of structure sizes in order to obtain more powerful and cost effective products; electronics and data storage. However,

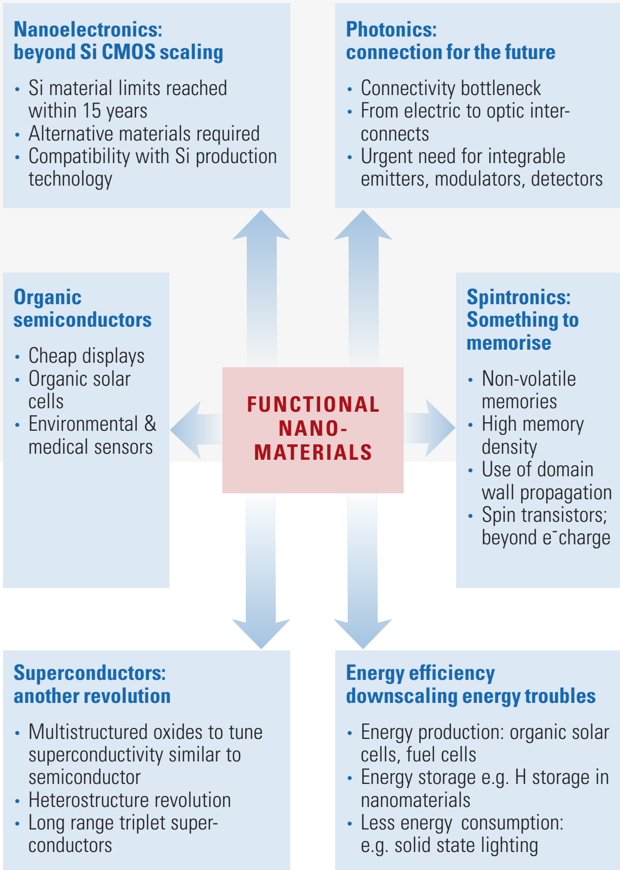

Fig. 5.13.2: Targets for future technology needs.

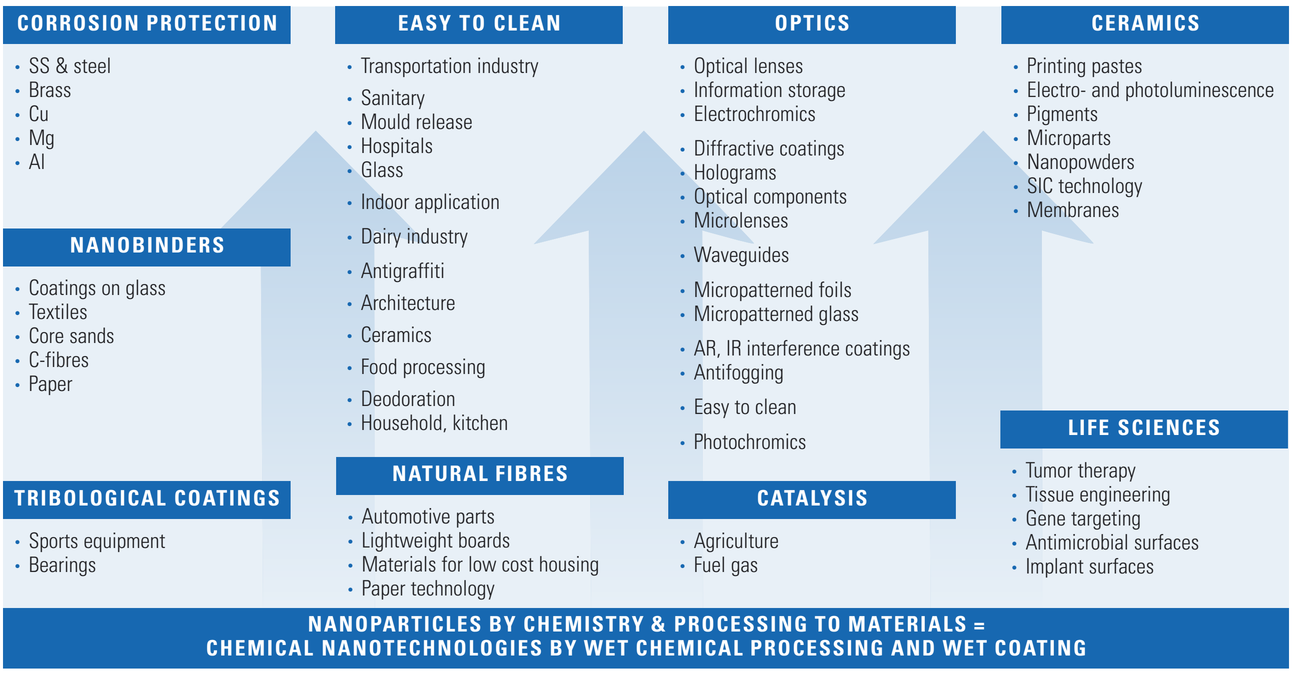

Fig. 5.13.1: Potential application areas for nanotechnology.

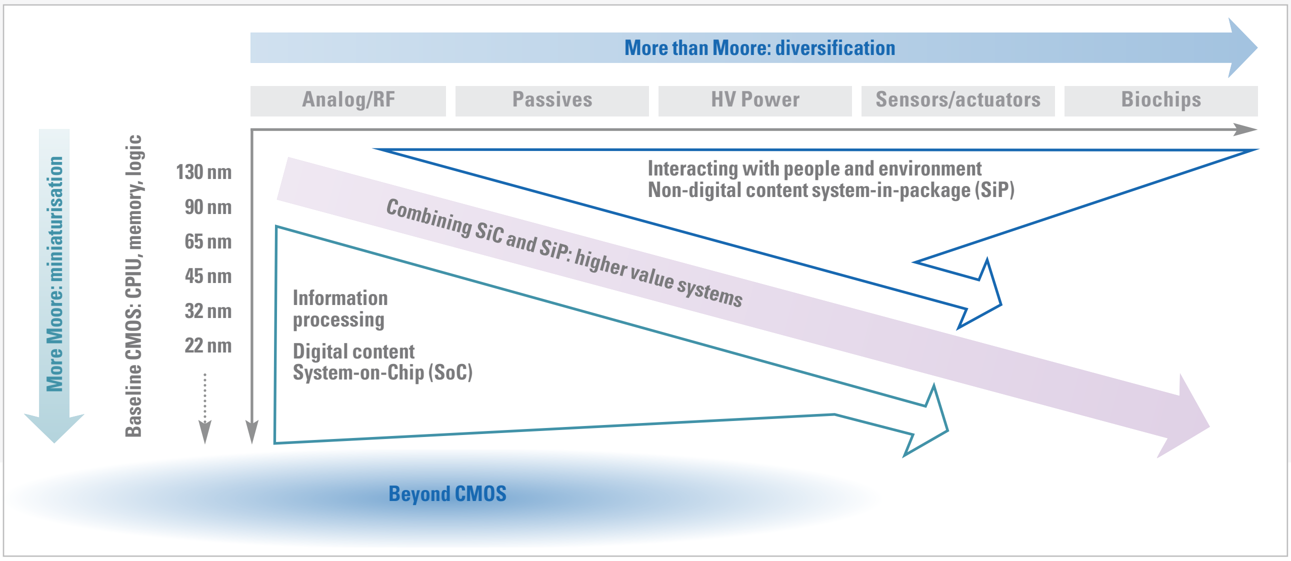

Fig. 5.13.3: Moore's law and More than Moore concepts.

the current technologies will meet barriers in the near future, and a better knowledge of size effects at the nanoscale is mandatory to achieve further progress.

The physical limits of downscaling CMOS technology of nanoelectronics are rather undefined. New scenarios must be developed for the introduction of new technologies (Fig. 5.13.3).

- To further improve the performance enhancement by effective downscaling processes: continuation of Moore's law to cope for modern world's demand of faster, smaller, cheaper and more efficient information technologies;
- To add new functionalities to current integrated circuit technologies: More than Moore;
- To open completely new directions like spintronics and molecular electronics with new concepts. (Beyond CMOS) and for developing new information processing technology after CMOS.

It is within the context of downscaling that scattering and spectroscopy with synchrotron radiation and neutrons will play a key role in the nanoscale research field:

(i) Material characterisation: One of the main challenges is the local resolution, in extreme cases down to single atoms, in order to monitor the structure and/or the dynamics of processes on various time scales e.g. chemical reactions or spin dynamics. The in-situ monitoring offered by synchrotron radiation will be an important asset in order to perform structural characterisations and measurements of properties during the fabrication of new materials and the operation of devices.

ii) Materials processing on the nanoscale require resolution and precision. In the technological development synchrotron radiation and neutrons may serve as an important tool for the future processing of materials and devices, e.g., for lithography beyond the

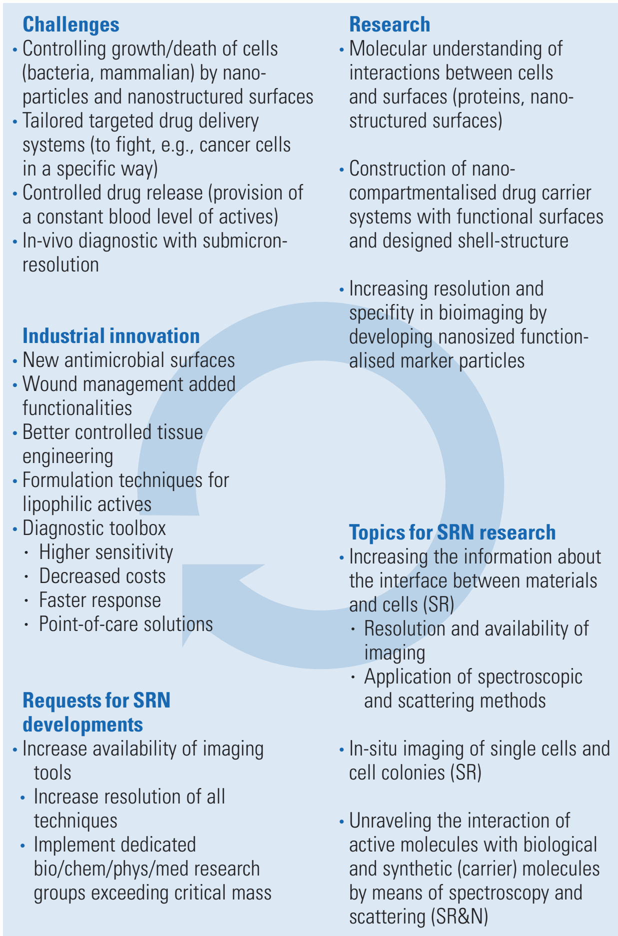

Fig. 5.13.4: Challenges and research needs for breakthroughs in nanotechnology for medicine and health.

optical limits. Neutron transmutation doping (NDT) of silicon-based nanostructures may gain increased importance for creating functionality on the nanoscale by controlling the spatial distribution of phosphor impurities.

iii) **Nanomaterials demand further development of adequate instrumentation.** It can be foreseen that synchrotron radiation may be used for calibration purposes". Both, synchrotron radiation and neutrons are being developed for extreme chemical and isotope sensitivity, for extreme spatial and time resolution, and for the analysis of new quantum states in nanostructures.

Medicine and health

The medicine and life-science applications may prove to be the most lucrative markets for nanomaterials technologies in the future. The challenges and research needs for breakthroughs are summarised in Fig. 5.13.4.

Nanocatalysis

The Grand Challenge for nano-catalysis science is to achieve an "atom-by-atom, molecule-by-molecule, nanounit-by-nanounit" understanding of how:

i) to design catalyst structure and
ii) to control catalytic activity and selectivity.

through efforts that involve both experiment and theory, we must develop a fundamental atomic-scale and nanoscale understanding of nanocatalysis.

The ambition is not only to synthesize selective and active heterogeneous catalysts with uniform and well defined micropores and catalytically active clusters, but also prepare them with a chemical composition and morphology so that they are stable and of long lifetime, when applied in the often hoarse environment of the industrial process.

Further research for heterogeneous nanocatalysts is needed in many industrial sectors. It may vary from large scale bulk processes in (petro) chemical industry, to automotive small scale applications as the exhaust catalyst beneficial to the environment. Fig. 5.13.6 gives an overview of the nanomaterials research needs in future innovations.

Overview nanomaterials in catalyst industries using synchrotron radiation and neutrons

To control the chemical and structural transformations of catalyst syntheses and its activation under reaction conditions, in-situ in solution or gas phase; from atomic to nano- and mesoscale; synchrotron and neutron irradiations are vital. Fig. 5.13.5 highlights the use of nanomaterials and the importance of synchrotron radiation and neutrons in the chemical-, transport-, energy and related industries.

Future developments will be needed in solid state heterogeneous catalysis. Important new processes foreseen relate to natural gas and liquid fuel processes, hydrogen production and storage and in the field of exhaust treatment and fuel cell technology. There are many important developments in chemical- and petrochemical technologies that require the development of new catalytic systems. Most important are miniaturisation activities to develop reaction systems on chips in the future probably of major use in fine chemical production and environmental catalysis.

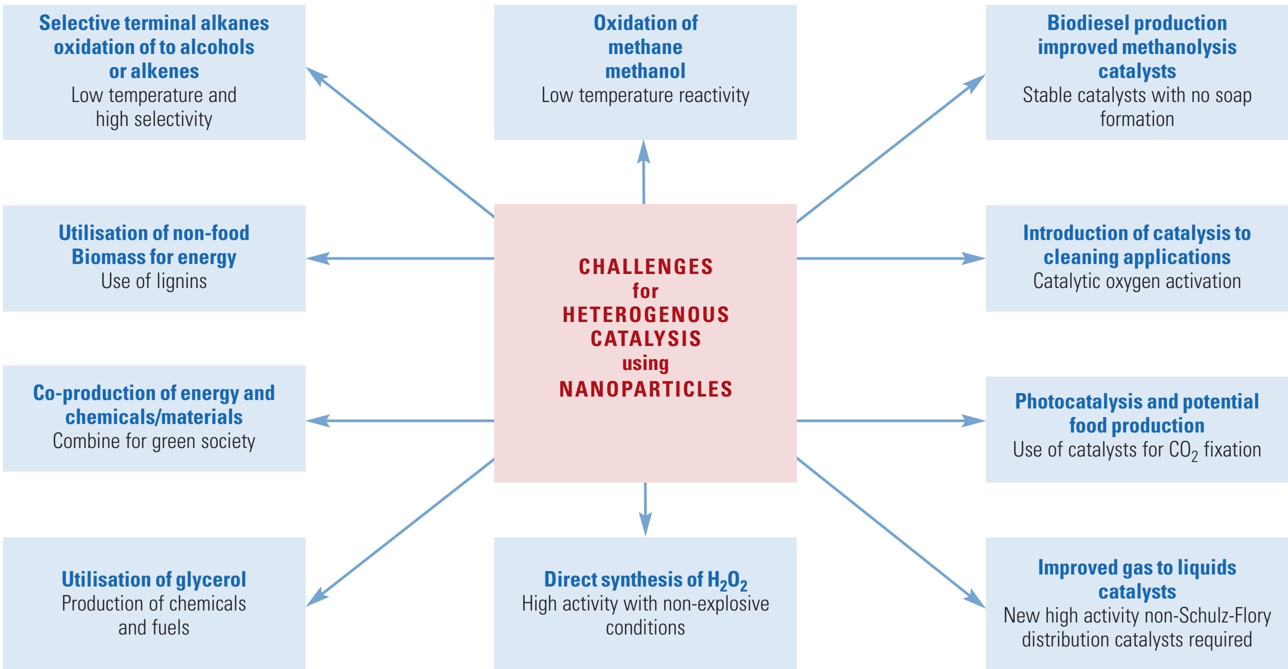

Fig. 5.13.5: Spectrum of nanomaterials in catalyst industries.

INDUSTRY SECTOR	RESEARCH PRIORITIES	KEY BARRIERS	POTENTIAL BREAKTHROUGHS	IMPACT OF SYNCHROTRON X-RAY AND NEUTRON TECHNIQUES
Refining, energy and transport	Structure-activity relations Catalyst for hydrogen production, solar cells and bio-fuel New materials for improved hydrogen recovery Efficiency of fuel reformers Catalysts for reduction of SO_2, NOx.	Global structure: crystallographic phases, composition, morphology, disordered and defects structure aggregate, clusters and colloids in powders and solutions Local environment: elemental and oxidation-state resolution Determination of adsorbate-substrate interactions, intermediate species, products Electronic structure and electron transfer in chemical reactions	Hydrogen storage capacity Effective hydrogen release Reduced gas emissions Increased renewable energy production Fuel cell technology	X-ray and neutron diffraction: in-situ measurements of samples embedded in electrolytes or biological solutions, inside heated or pressurized cells, and under oxidizing or reducing atmosphere EXAFS, XANES and neutron diffraction, spectroscopy using isotopic substitution
Bulk chemicals, polymers and materials Fine chemicals and pharmaceuticals	Catalyst deactivation Selectivity New catalyst materials High yield catalysts Ligand design and synthesis Catalyst immobilisation Modelling	Global kinetics	Increased selectivity Alternative feed stocks Reduced energy consumption High performance materials Polymer based solar cells and electronics	Vibrational fingerprints via IR and neutron vibrational spectroscopy; core level shift via XPS and NEXAFS UPS; valence band; XES: atom-specific density of states; electron yield spectroscopy; laser-induced femtosecond dynamics
	New catalysts New synthesis routes Parallel and combinatorial screening and testing methods Biocatalysts (functional genomics) Modelling	Trace-element analysis Surface chemistry; molecular diffusion Chemistry: nanostructure relation Structure: chemical function relation Multidimensional imaging	Hydrocarbon valorisation Reduced time to market Waste reduction More complex chemicals High purity chemicals	Nondestructive non-invasive and quantitative measurements; high-floux sources; real-time studies of global kinetics of catalytic processes Neutron activation analysis; X-ray fluorescence analysis Neutron-quasi-elastic scattering Real-space and reciprocal-space scattering Element contrasting, isotope replacement, hydrogen substitution Concurrent in-situ measurements of spatial, chemical, temporal properties on one beam line

Fig. 5.13.6: Catalyst technology – research priorities and key-barriers in different industrial sectors.

Nanotechnology in the chemical industry
- Synthesis of nanoparticles and nanostructured materials
- Nanomodification of surfaces
- Formulation of nanostructures

High radiation x-ray and neutron sources
- Advanced and fast imaging
- Scanning and time-resolved scattering
- High-resolution spectroscopy

Needed
- Structure property relationships
- High-throughput screening

Provided
- Structural insight
- Fast characterisation

INNOVATIVE AND FAST DESIGN OF

Nanomaterials, nanosurfaces, nanoformulations with new and improved properties for sustainable growth

Fig. 5.13.7: Interaction of nanomaterials research needs and the role of synchrotron radiation and neutron experiments.

Nanomaterials in the chemical industry

Fig. 5.13.7 bridges the gap between nanomaterials research needs and the role of synchrotron radiation and neutrons to create innovative products in the chemical industry.

Energy technology

In Europe, there is a pressing need to develop energy sources in order to reduce dependency in fossil fuels and other sources harm to the environment. Promising technologies for solar energy, hydrogen fuel cells, solid state lightening, supercapacitors, rechargeable batteries, and improved nuclear power will have to play critical roles, but fundamentally new scientific approaches are needed. Discovering, exciting developments and understanding of new nanomaterials science are uniquely positioned in overcoming many of the technical barriers to energy security. Cutting edge science will strongly influence developments in energy conversion, energy storage, and end-use energy efficiency. An overall picture of the future directions for research is given in Fig. 5.13.8.

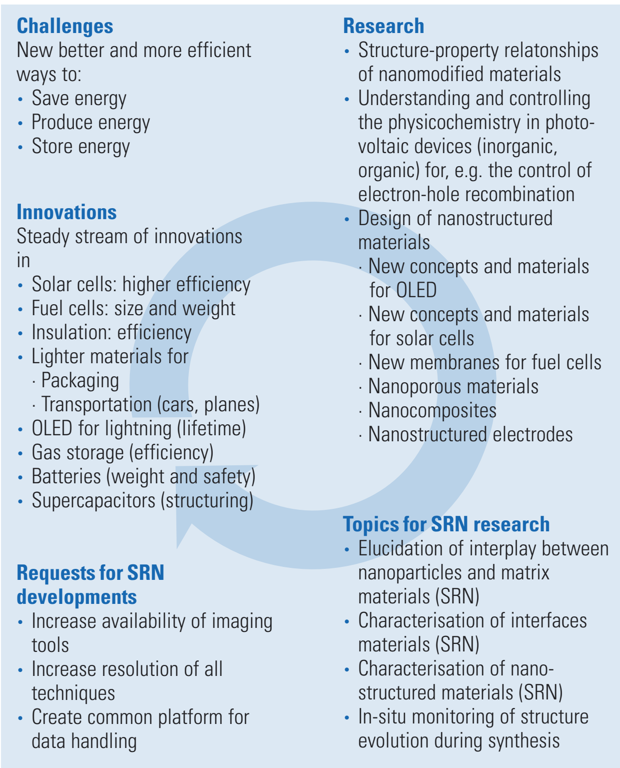

Fig. 5.13.8: Future direction for research for energy technology.

The requirements that will drive the development of new synchrotron radiation and neutron based research facilities for new energy technologies are: Fig. 5.13.9.

- Increased structural resolution – to elucidate the atomic, nanoscopic, and mesoscopic arrangements that are crucial for enhanced performance; scattering methods for Fourier space imaging;
- Increased spatial resolution – to directly image the functional units in physical space;
- Increased chemical resolution – to unveil the oxidation and binding state of the elements involved in the conversion process under investigation;
- Increased time resolution – to monitor in real time the processes involved in the activation and deactivation of the novel energy converters.

Pursuing these four goals in parallel (albeit, in part, in a task sharing mode between different facilities) will represent an extremely challenging task, which may correspond to the development of a new generation of synchrotron and neutron sources. Although demanding, the provision of such powerful tools will without doubt pay off in terms of substantial advances towards a more sustainable energy system.

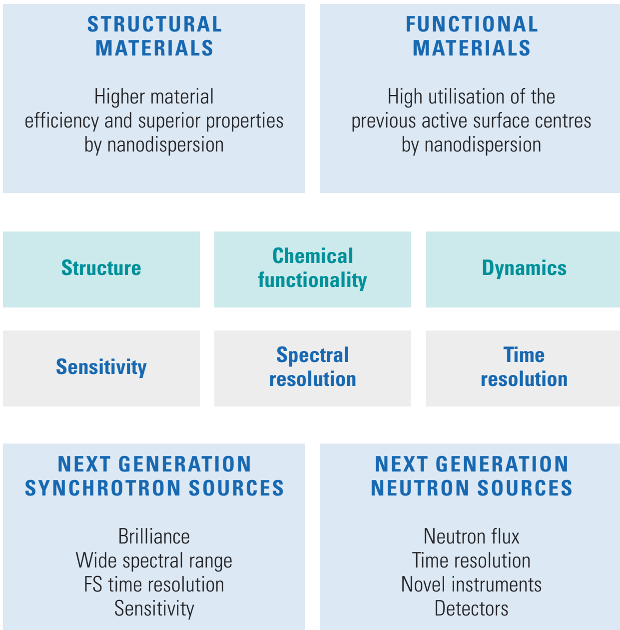

Fig. 5.13.9: Needs for developments at large-scale facilities to comply with new energy discoveries.

Nanotechnology and food

It is clear that nanotechnology will have an impact in the field of food technology. However, given the fact that consumer concerns, at present, about the direct application of synthetic nanomaterials in food are strongly developed, the major impact will come mostly from methods and tools rather than from a direct application of nanotechnology in the design and making of food. The most important fields are summarised in Fig. 5.13.10.

Nanodiagnostics aim to develop cheap and highly integrated diagnostic systems of higher sensitivity, specificity and reliability for chemical, biological and medical analysis.

Nanomaterials will play a major role in the form of nanocomposites in packaging and protective coatings (improvement of barrier properties). Furthermore, "intelligent materials" might be used for food monitoring (integrated quality indicators alerting a consumer about contamination and/or presence of pathogens, invisible nanotags for product traceability).

Nanotools (e.g. atomic force microscopy, electron microscopy, neutron, x-ray and light scattering techniques) are indispensable instruments for us who allow analysing and understanding the complex molecular architecture and behaviour of proteins, polysaccharides, lipids, food colloids and their structuring principles in the context of complex food matrices. Particularly important are possibilities that future next generation large-scale research centres (synchrotrons, neutron spallation sources) will be able to offer in order to perform in-situ and time-resolved studies under processing conditions.

Nanodelivery will aim at creating novel delivery systems parallel with developments in nanomedicine (key word "functional food"). It is the area where consumer concerns have to be considered strongly.

The research field is in its infancy and efforts are thinly spread over many research institutes and universities throughout Europe. To realise an impact, for the welfare of the future society, there is a need to concentrate the research activities in Europe.

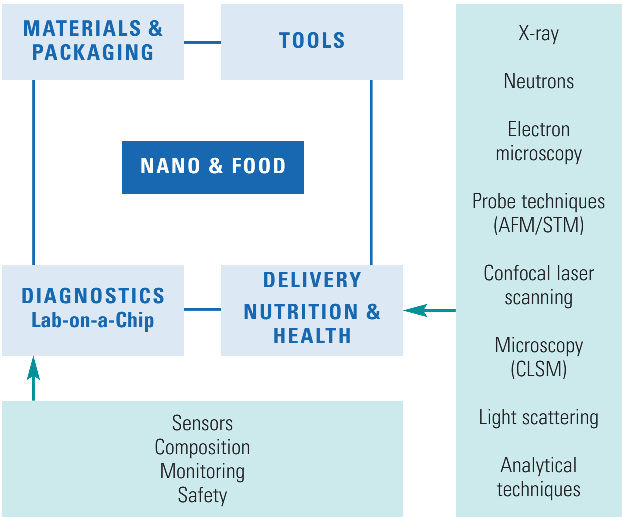

Fig. 5.13.10: Challenges for synchrotron radiation and neutron research on nanomaterials in food.

Conclusions and recommendations

Effective utilisation of synchrotron radiation and neutron resources, and further smart developments of these resources, will bring new insights into nanoscale phenomena and properties that will impact diverse application areas such as catalysis, photovoltaics, fuel cells, membranes, coatings, displays, ceramics, thermoelectrics, adhesives, sensors, batteries, pharmaceuticals, and magnetic and semiconducting devices.

"Physics-related technologies" such as nanoelectronics and nanomagnetics have already established close contacts with large-scale facilities but efforts should be strengthened. It is of vital importance to create a mechanism in Europe to bring the nanomechanical technical centres and engineering industries such as transport, energy, security, environment closer in contact with the synchrotron radiation and neutron facilities. This will require twofold efforts:

i) Large-scale facilities should take actions to create a friendly environment for these science and technology branches and install nanomaterials science platforms for these new sciences besides the established physics and pharmacy communities.
Ii) The European Commission, national- and European funding agencies and governments and industrial groupings should take initiatives to promote the bridging between industry – research and large-scale facilities by stimulating European research and development programmes on nanomaterials using the large-scale facilities. GENNESYS could be a good mechanism to realise this objective.

It is recommended to set up an international experts committee to explore the potentials and work out a proper strategy.

6. METROLOGY, STANDARDISATION, INSTRUMENTATION – NANOMATERIALS TECHNOLOGY – THE NEED FOR NANOMETROLOGY RESEARCH AND TECHNOLOGY

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Micro- and nanostructured materials frequently exhibit new material properties as compared to their bulk counterparts. As a result, the design and the production of nanostructures are of large importance in order to create materials with new properties and functions. In recent years, novel properties have been discovered and exploited in many different areas.

If the structures are, in at least one dimension, in the order of a few nanometres, quantum confinement effects for the electrons become important. As a result, the electronic. magnetic and optical properties are altered, affecting material characteristics such as band gap, conductivity, magnetic or optoelectronic activity. Such materials are thus of importance in electronics, optoelectronics, spintronics and magnetism, i.e. electroluminescing silicon nanostructures, thin metal films exhibiting giant magneto-resistance, carbon nanotubes with configuration and diameter-dependent bandgaps or luminescent semiconductor nanocrystals.

Structure sizes of a few hundred nanometres are comparable to the wavelength of visible light or adjacent spectral regions. As a result, optical properties can be directly tailored by nanostructuring/microstructuring on this length scale, resulting in applications such as optical waveguides, interference coatings for optical elements, photonic bandgap materials or optical metamaterials with negative permeability and the resulting exotic optical properties.

While electronic and magnetic properties are modified by patterning on the scale of a few nanometres and optical properties are modified by patterning the structures from about 1/10 of the light wavelength to several wavelengths, mechanical properties are influenced over a wide range of structure sizes. Starting from the strengths of individual bonds, it is the texture and structuring over the entire nanometre and micrometre range that determines mechanical properties such as the Young's modulus or the shear modulus. A specific topic is the hierarchical composition of nanotube yarns or biological tissues, where fibres and crosslinks on the nano- and micrometre scale produce specific macroscopic mechanical properties. Nanoelectromechanical systems (NEMS) integrate nanosized mechanical parts with electronics for applications in mass or force sensing and imaging. Other mechanical phenomena such as the wettability of a surface by water can be influenced by patterning with structure sizes from sub-micrometres to tens of micrometres, as exemplified by self-cleaning surfaces.

Modern composite materials are structured and inhomogeneous on various length scales. In compound materials, one combines complementary benefits of the components aiming towards a new material with hitherto unknown properties. In this area of nano-emergent materials, understanding and control of the properties and functionality of the compound materials therefore demands microscopic characterisation and control of the composition and structure from the atomic scale. This can be on the nanoscopic scale, well into the micrometre

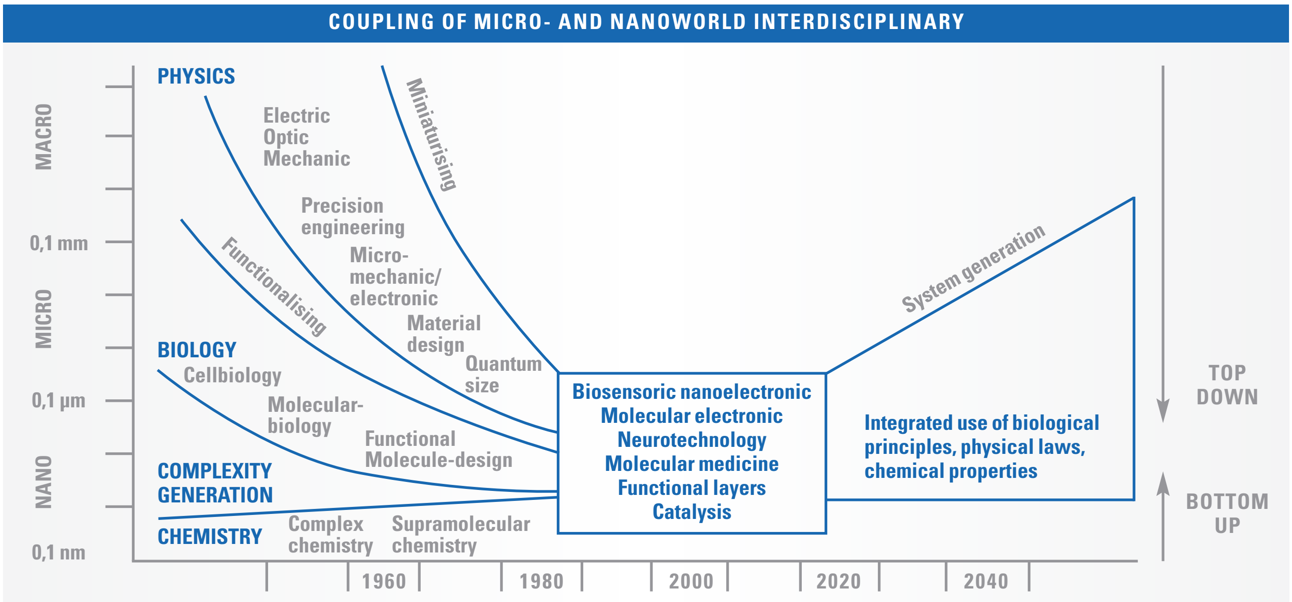

Fig. 6.0.1: Meeting of sciences and coupling of the micro- and nanoworld.

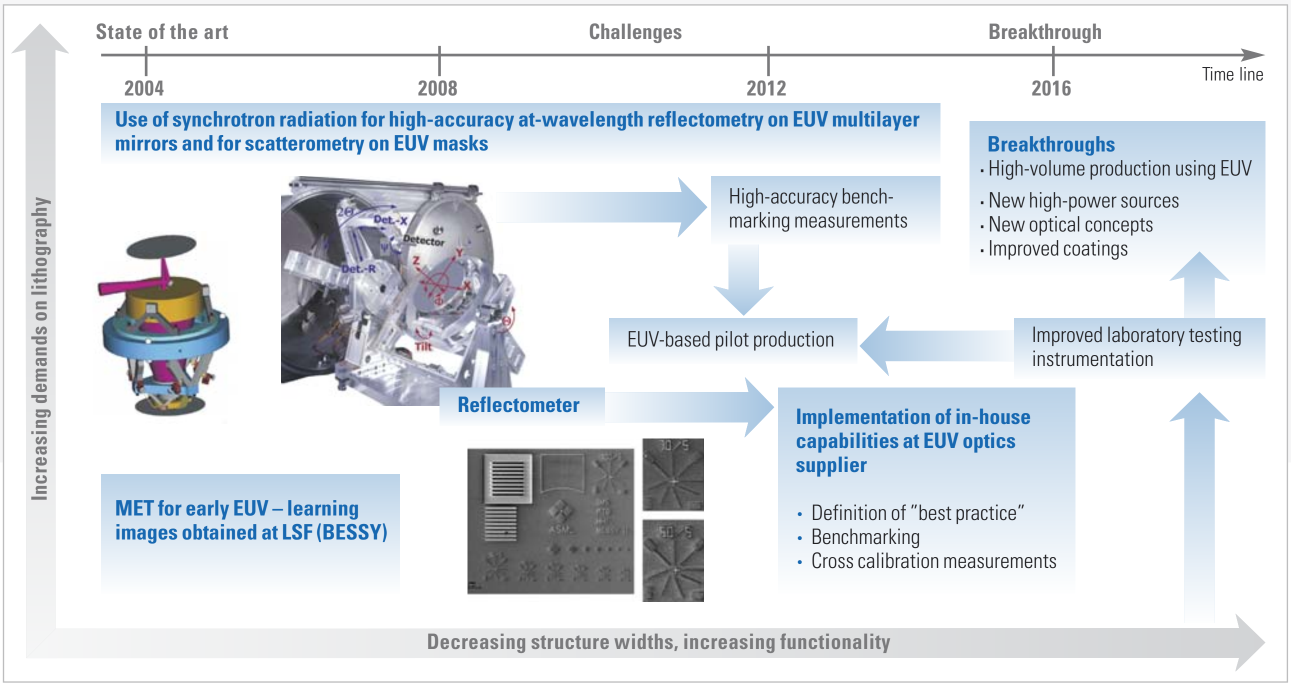

Fig. 6.0.2: Roadmap for standardisation of nanometrology: "lithography".

regime. For the reproducible production of these materials, metrology for the process control and standard reference materials are required.

The interplay of the various scientific disciplines and technology is illustrated in Fig. 6.0.1. Nanomaterials will show new interesting functions for new products with reduced production costs, longer lifetime, etc.

In addition to utilising mechanisms of self-organisation for the production, patterning processes by electron and ion beams as well as x-rays, offer the chance to control and modify the relevant materials parameters with unprecedented accuracy on the nanometre scale. This is already realised on the (sub-)micrometre scale in the production of micromechanical parts (LIGA). In the near future, it will be realised in the industrial production of semiconductor electronic devices (EUV lithography). Fig. 6.0.2 shows a typical roadmap for the development of lithography of nanomaterials.

6.1. GRAND CHALLENGES FOR NANOSCALE METROLOGY, STANDARDISATION AND INSTRUMENTATION

The grand challenge for a reliable production is to develop the ability to reliably and reproducibly image and measure any nanostructure for any relevant property with atomic accuracy in three dimensions. Realising the potential of the emerging nanotechnology industry will require the following:

- High performance, cost-effective, reliable instrumentation;
- Improved measurement methods (metrology);
- Information and data transmission and interpretation;
- Globally-accepted standards for measurement;
- Identification of properties and structures at the nanoscale.

Accurate measurement of dimensions, characterisation of materials, and elucidation of structures at the nanoscale will be critical to the future commercial development of nanoscale materials and devices. However, in most cases a combination of various probes is necessary to get a whole image of the properties of the sample under investigation (Fig. 6.1.1). Due to the size and the large surface to volume ratio instruments with high spatial resolution have to be improved in their sensitivity or combined with such surface analytical instruments which are based on electrons, photons, ions or neutrons.

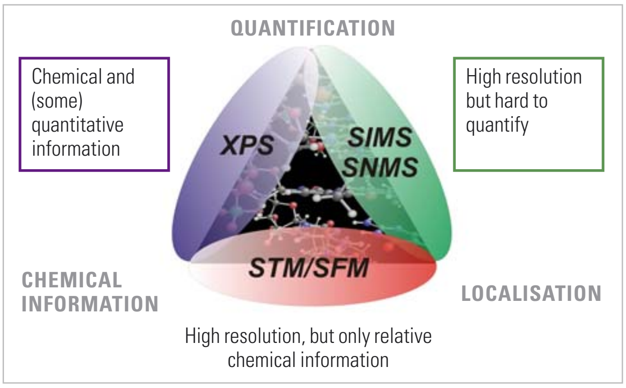

Fig. 6.1.1: Information obtained by different techniques, each measure its own physical or chemical quantity.

Due to the large penetration depth, the scattering of neutrons or synchrotron radiation allows for unique insight into the structure of materials including biological systems. In addition, one is able to investigate the sample under extreme conditions such as high pressure, low temperature or high magnetic fields. Tomography, microscopy and holography provide direct images of individual selectable nanostructures with, at present, a resolution down to a few nanometres exploiting different contrast mechanisms. X-ray spectroscopy gives direct insight into the electronic structure, magnetic properties and geometry in an element-specific and localised manner. X-ray and neutron scattering techniques, on the other hand, provide precise statistical data concerning the median values as well as the range of deviations measured for an ensemble average of nanostructures. For these reasons, in the U.S., all the five nanomaterial centres recently established by the DOE are located in close proximity to a synchrotron and/or neutron source.

Concerning laboratory instruments, most of these are at the resolution or detection limits (e.g. surface analytical instruments see Fig. 6.1.2). Here, only TOF-SIMS or Dynamic SIMS reach the physical limits given, but destroy the sample under investigation.

Chemical information, however, is only one of the aspects needed for characterisation. In order to acquire the necessary knowledge, one must know more than a material's chemical components. Information has to be provided about the inner and outer structure, the amount of chemical elements, etc., and their respective dependencies on the time or environmental conditions. For example, nanoparticles necessary for catalyst reaction must be characterised for the internal structure and outer shape. Therefore, a combination of measurement techniques is necessary to address nanotechnology challenges. This could be established or alternatively, new techniques can be developed which fulfill the requirements related to the measurement task and its condition. The instrumentation and the measurement quantity will require calibration of the instrument by standard specimen and guidelines, neither of which are available when using the established metrology. However, the amount of data to be handled with experimental and theoretical investigations would be much greater than what is currently done. In addition, we have to merge the results of experimental as well as theoretical investigations in order to improve our knowledge. Using separate tools for measurements and the subsequent merging of data requires the full insight in the physics of nanostructures to ensure that no artefacts are generated in the measurement system.

As new nanomaterials, structures and devices are fabricated, assembled and manufactured into usable products, standardised improved instrumentation and metrology will be vital for providing quality control and ensuring reproducible performance. Recently, there has been a dramatic improvement in our ability to measure, characterise, visualise and manipulate matter on scales that could only be imagined a decade ago. However, there are still significant challenges in metrology and characterisation which, if not overcome, will hamper our ability to discover and commercialise new nanostructured materials, nanoparticles and nanocomposites with novel end use properties. This requires the development of new metrology instrumentation and infrastructure for both laboratory research and nanomanufacturing.

This is confirmed by a recent survey on the potential of nanomaterials for future products [European Survey on Success Factors, Barriers,

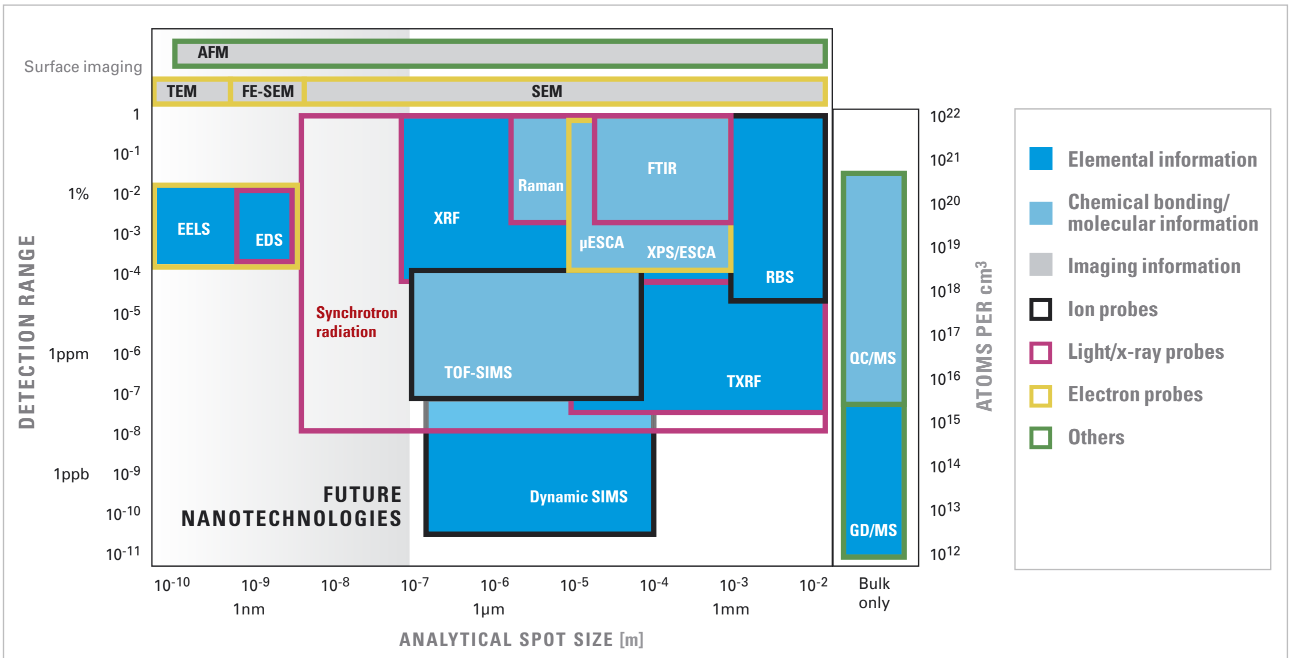

Fig. 6.1.2: Elemental analysis techniques – detection range, sensitivity and lateral resolution.

and Needs for Industrial Uptake of Nanomaterials in SME's, Nanomaterial Roadmap 2015, Coordinator: Steinbeis-Europa-Zentrum, Karlsruhe, July 2005]. It points out that the main factors for successful operation of companies already working with nanomaterials are:

1. Material properties (78%)
2. Quality improvement (47%)
3. Cooperation with other companies (37%)
4. Cooperation with R&D organisations (33%)

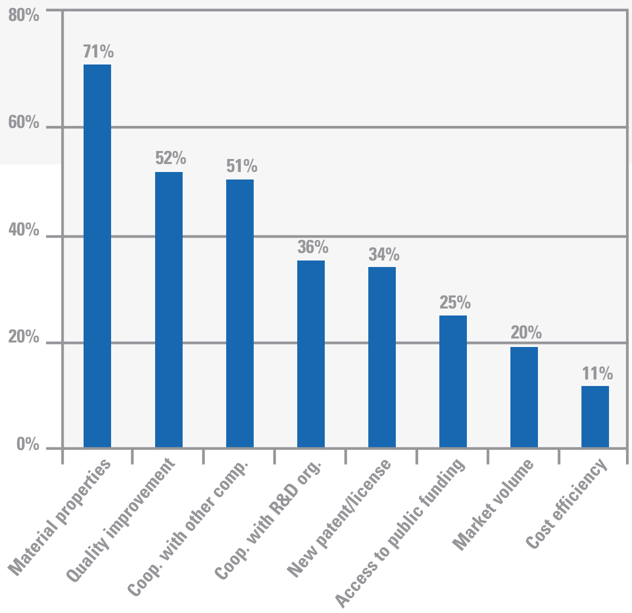

Fig. 6.1.3: Specific success factors for companies presently working with nanomaterials on the medical & health market.

Improving the quality of products is directly related to the competition advantages. This is a challenging process on the nanoscale. Important for the success of companies is the cooperation with R&D organisation during the development phase. However, as for other companies on the market for nanotechnology companies, production process technology and price/performance are the main barriers for the application on the market. An additional bottleneck is the lack of knowledge transfer from scientific organisations to SME's and the relation of nanoscience results to usable applications (see Fig. 6.1.3).

Instrumentation and metrology are both essential for an emerging nanotechnology company and necessary for successful competition on the European and worldwide market. Investigation of new properties of nanostructures will be made at the highest research level possible. But this could be not the basis for production; a new technique should fulfill more conditions. Aside from the knowledge transfer to companies, it requires the highest effectiveness of measuring systems (see Table 6.1.1). Here, nanometrology has to be understood as a support for the linkage between research-oriented and industrial-oriented needs.

It will be a significant challenge to adapt the instruments developed for scientific research to "fit for purpose" industrial instrumentation. This means particularly that the metrology approaches of this exploratory nanoscale research have to be based on common principles of traceability and consistency (see Fig. 6.1.4).

RESEARCH-ORIENTED	INDUSTRIAL NEEDS
Requires highest precision possible	Requires highest effectiveness of measuring systems
Vision driven observations	Reliable products, i.e. quantitative parameters of products should be within tolerances
Quantity of measured parameters – as many as necessary	Quantity of measured parameters – minimum acceptable for reliability
Measurement time and cost – are not important	Measurement time and cost should be minimised, if necessary online and/or in-situ techniques
Almost ideal measurement and environmental conditions	Day-to-day reproducibility in a production environment (conditions affected by vibration, air pollution, temperature variations, etc.)

Table 6.1.1: Aspects in research and industry.

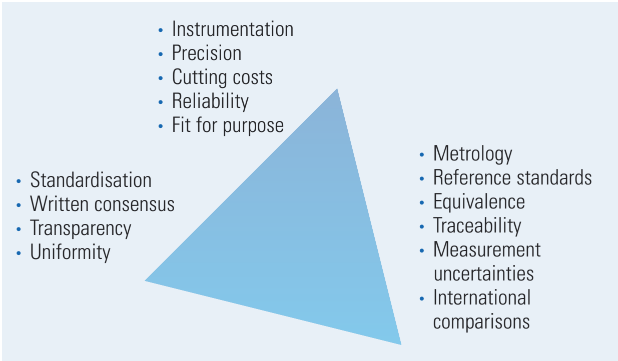

Fig. 6.1.4: Triangle of standardisation, instrumentation and metrology.

Entirely new metrology tools and analysis will be required to meet the needs of the emerging nanotechnology industry. While much progress has been made, current instrumentation and metrology are at their limits and much greater capabilities will be required, from laboratory to commercial scale manufacturing. Revolutionary advances will be necessary to support an emerging and potentially exceedingly large nanotechnology industry.

Thus, in order to close the gap between research and industry, the general nanometrology should provide:

- Validated measurement techniques including investigation of measurement uncertainty;
- Approved theoretical models and computing techniques to get insight of details beyond the experimental observation limit to clarify the limit of uncertainty due to probe – sample interactions;

- Virtual or network based techniques to provide virtual instruments for an improvement of uncertainty calculation, e.g. a virtual scanning probe microscope;
- Improved strategies for the probing of physical quantities in a production process using minimised measurements; i.e. how to conclude results from measurements of a small number of single particles to a large variety in the production process;
- Internationally verified standards related to the measurement tasks for nanoscale structures and interactions;
- Reliable parameters for new materials and/or standard reference materials to calibrate and test instruments;
- Strategies to convert time-consuming high level expert measurements to computer-controlled on-line measurements by using standards selected by "material property needed" with small uncertainty, improving measurement techniques to allow for small bandwidth detection of material properties, etc.

The above should be realised in the form of roadmaps. These roadmaps should be defined by experts for nanotechnology industry needs for the next 5 to 10 years. Progress should then be reviewed every 2–3 years, with goals and guidelines redefined accordingly. Such roadmaps should provide information about the development and the direction for nanotechnology for industry, the manufacturers of instruments, and metrology institutes.

This "procedure" has been confirmed to be very successful in the case of the International Technology Roadmap for Semiconductors (ITRS) and the Chemical Industry Research and Development Roadmap. Both give trends and emphasise metrology and advances in instrumentation as key enabling technologies for emerging nanomaterials and systems, citing specific needs in real-time analytical and characterisation tools, including standardisation and informatics. However, compared to semiconductor technology, nanotechnology has a much broader scope of applications in various fields of physics, chemistry, and industry.

The build-up of educational programmes is also of utmost importance and it will be necessary to upgrade university facilities and create a multidisciplinary research community for metrology at the nanoscale. Education and training opportunities should be pursued to create the skilled workforce needed to support nanotechnology, from basic characterisation of properties to fabrication and manufacturing.

Instrumentation and metrology (the science of measurement) will provide an important basis for the emerging nanotechnology enterprise. Globally accepted standards for measurement and identification of properties and structures at the nanoscale will be needed to ensure that European countries can compete with their nanoproducts in the international marketplace. In addition to the geometrical dimensions and structures, local atomic/electronic/optical/magnetic properties must be characterised for a functional understanding of nanomaterials and systems.

6.2. NANOMATERIALS – KEY CHALLENGES FOR CHARACTERISATION

In support of nanomaterials development to revolutionise functional materials technology, it will be essential to create reliable standard reference nanomaterials and nanostandardisation protocols. Fundamental research and development will be required to deliver the basic technology for ultrafine and high precision measurements to ensure reliable reproducibility and reliability of the product. As we are today lacking these standard materials and metrology protocols, companies are calibrating measurement tools using in-house standards, which are of variable accuracy, and may not be agreed across industry. What is needed are methods capable of sub-1 nm repeatability and nanometre accuracy for use in nanoelectronics and nanomanufacturing metrology and process control (Fig. 6.2.1).

Nanostandardisation and standard reference materials (SRMs) are required in support of nanocharacterisation across the fields of nanomechanics, nanoelectronics, nanofabrication and nanomanufacturing. Nanostandardisation is needed in small-angle x-ray scattering and small-angle neutron scattering as they undertake critical dimension metrology of nanoscale structures. These are essential to quickly, quantitatively, and non-destructively measure the smallest, or 'criti-

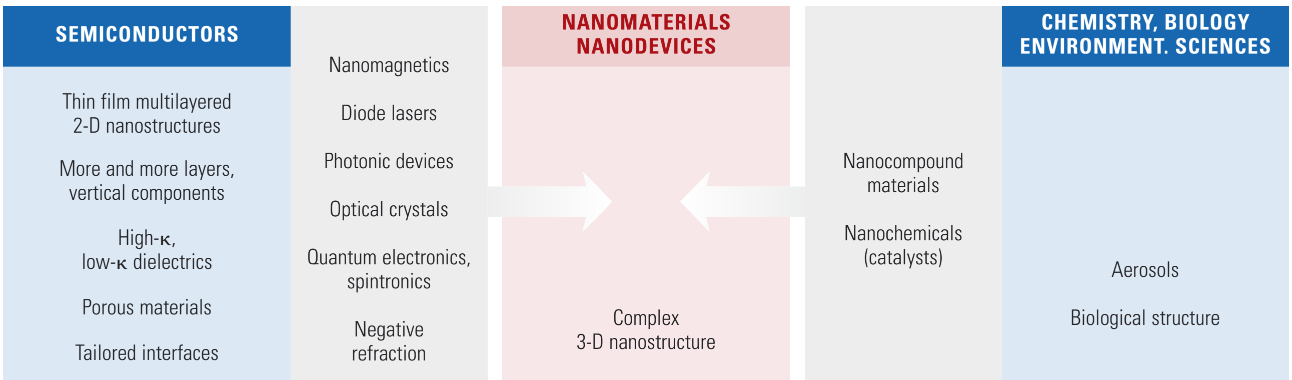

Fig. 6.2.1: Overview of potential development paths for nanomaterials and devices.

cal,' dimensions with subnanometre precision. It should be mentioned that the microelectronics industry is currently testing a wide variety of porous low-dielectric constant, 'low-κ', materials for future use in integrated circuits. To understand low-κ thin film properties, and in order to tailor the nanoporosity for performance, a quantitative analysis of pore size distribution is vital.

The ability to measure trace chemical composition at surfaces and interfaces depends on the spatial-resolution capabilities of measurement technologies. Nanostandardisation is needed for the development of high-intensity hard x-ray nanoprobes to assist industry in attaining ultra-high-resolution chemical and depth profiles:

- The development of standardised nanometre-probe x-ray photoelectron spectroscopy is needed to trace electronic inhomogeneities in materials over near-surface depths.
- The characterisation of thickness of dielectric layers requires sensitivity to 1 nm and, and can be achieved with the further development and standardisation of grazing incidence x-ray photoelectron spectroscopy to quantify the thickness and chemistry of ultrathin gate dielectric layers in a non-destructive manner.
- The grazing incidence small-angle x-ray scattering and diffraction need to be extended to address low-dimensional multifunctional materials such as multi-ferroic nanodot arrays.

Successful realisation of an x-ray enhanced scanning tunnelling microscope (STM) will couple atomic-scale spatial resolution with element sensitive imaging for atom-based dimensional, chemical and electronic metrology.

6.3. NANOTOOLS – KEY CHALLENGES FOR ANALYTICS

Recent developments in nanoscience and technology cover an extremely wide field of applications and respective needs for measurement capabilities (see Table 6.3.1). Correspondingly, the research needed for new metrology methods is indicated for almost all fields of metrology in the roadmaps developed in this GENNESYS White Paper.

Optical measurements using photons as probe are used in almost all high-accuracy dimensional measurements. This is mainly due to the

NANOCHARACTERISATION OF FUNDAMENTAL MATERIALS PROPERTIES	STRUCTURAL NANOMATERIALS	FUNCTIONAL NANOMATERIALS	NANOFABRICATION
Realisation of nanoscale 3-D imaging capabilities	High throughput automated nanomechanical measurements: multi-functional, high spatial resolution, rapid nanomechanical measurement and analysis	Nanoelectronics Instrumentation and metrology for advanced CMOS	Instrumentation for nanofabricated structures, mass production, reliable, reproducible, fast and accurate measurement technology for production applications
Rapid acquisition of nanoscale data	Integration of multiple testing techniques in nanomechanics	Instrumentation and metrology for emerging novel devices	Interconnectivity of macroscopic and atomic length scales
Sample preparation and handling		Nanophotonics Synthesis for nanophotonic devices	Control of the three-dimensional synthesis of nanostructures
Characterisation of surface and interface phenomena – also in-situ	Nanomechanical measurements: rapid, accurate, representative of the device or system environment in real time and length scales	Nanomagnetics	Real-time decision support for nanomanufacturing
Measurement of complex structures with compositional heterogeneity	Testing under industrial simulative environmental condition	Measurements of the magnetic properties of a cubic nanometre of material	"Real device" inspection with nanometre resolution
Combination of measurement capabilities: compositional and performance parameters to be quantitatively and reproducibly measured on the nanoscale	Standard test methods and calibration (Relevant to all areas, not just nanostructured materials)	Imaging of spin dynamics	Metrology for liquid phase manufacturing of nanomaterials
Qualitative measurement of dispersion of nanoscale substances in a matrix	Qualitative measurement of relevant material characteristics – electrical, magnetic, chemical, mechanical	Probes that decouple the measurement from the phenomenon	Production ready standards and metrology

Table 6.3.1: Measurement challenges for different fields of nanotechnology.

fact that photons are not deflected by electromagnetic fields (like e.g. electrons) and the photon-sample interaction is well understood. The whole measurement can be well described, permitting reliable and traceable dimensional measurements (see Fig. 6.3.1). The disadvantage is that the resolution for classical microscopy using visible and UV-light is limited by the wavelength. A driving force on this field is the semiconductor industry. At the moment, this is the pioneering high-volume industry for nanotechnology which produces highly complex objects with total dimensions in the cm-range and structures of only a few nm in height and several tens of nm in width. Many new applications in nanotechnology are based on semiconductor technologies (lithographic nanostructuring, thin layer deposition, etching processes, etc.). However, in future high resolution radiation sources (EUV) have to be used to produce the small structures, techniques which also are useful for other fields.

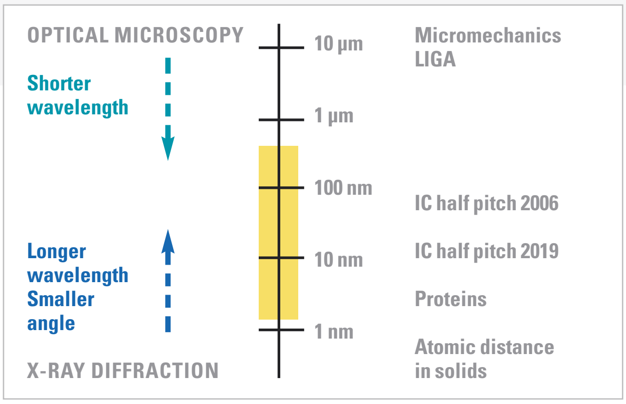

Fig. 6.3.1: Overview of objects and photon-based investigation methods in the nm-range.

For high-resolution applications, synchrotron radiation, neutrons, electron probes and more recently, scanning probe microscopy are used. Table 6.3.2 gives an overview of common techniques using photon, electron and force based techniques.

All the techniques above need to be improved further in order to fulfill the requirements for traceable measurements. For example, measurements at sub-nanometer precision are complicated by complex probe-sample interaction and surface effects. This has to be taken into account for absolute measurements. On the other hand, many techniques, however, will be intrinsically slow (nanobeam tomography, photon based scanning probe microscopy, ...) or for the time being, cannot be transferred to the industrial laboratory and production metrology due to a lack of appropriate photon sources i.e. tabletop type facilities.

However, compared to other probes, photons and neutrons are a very convenient probe for accurate and traceable measurements at nanoscale due to direct relationship to frequency and/or wavelength. The broad spectrum available at synchrotron radiation and neutron facilities provides a profound basis for the up-down and bottom-up

TYPE OF PROBE	OPTICAL PROBES (VIS-UV – EUV – X-RAY)	ELECTRON PROBES, TEM	MECHANICAL OR FORCED BASED PROBES (SFM)
Dimension Advantages	2-D to 3-D (l) · Well-understood, well-defined interaction of photons · Fast imaging technique · High penetration depth possible, depending on wavelength · Investigations of ensembles of particles	2-D to 2.5-D · High resolution down to atomic scale · Large interaction volume (SEM) small (TEM) smallest (STM) · Crystalline structure of surfaces (STM) and nanoparticles (TEM) · Investigation of single particles	2.5-D to 3-D · High resolution down to atomic scale · Type of probe-sample interaction used for imaging can be selected · Very short interaction length · Investigation of single particles
Issues	· Limited resolution with optical/ VU light · Unknown refractive index in UV/EUV range · Spatial resolution in elemental analysis (XPS, XRF, …) · Reduction of exposure time for biological materials · Reduction of carbon contamination if high energy light source is used	· High or ultra-high vacuum environment · Application to biological systems · Strong electron-sample interaction, partly difficult to model · Sample preparation only on surface · Elemental analysis (AES, TEM, EDX, EELS, etc) · Carbon contamination	· Strong probe-sample interaction, · Difficult to model only on surface · Slow scanning technique · Limited scan ranges
Further developments	· Imaging x-ray optics · X-ray tomography of single biological cells or nanoparticles or nanostructures	· Improved modelling of electron-sample interaction	· 3-D probing of surfaces of nanostructures

Table 6.3.2: Techniques most commonly used today for micro- and nanoscale imaging.

approach shown in Fig. 6.2.1. Moreover, synchrotron radiation measurements can also provide necessary information about local atomic/electronic/magnetic/ properties. This is the mandatory basis for a functional understanding of the behaviour of nanomaterials.

6.4. KEY CHALLENGES FOR SYNCHROTRON RADIATION AND NEUTRONS NANOMETROLOGY

Today the main tasks for synchrotron radiation based metrology are the (Table 6.4.1 and Fig. 6.4.1):

- Development of special equipment for measurements in the nanometre regime with special focus on traceability aspects of the measurements;
- Development of suitable models for estimation of measurement uncertainties;
- Development and characterisation of standard reference materials which can be transferred to industry.

To improve this and to establish synchrotron radiation and neutron in the field of nanoscale metrology, a lot of work has to be done. Key challenges for such a synchrotron radiation and neutrons nanometrology are to be solved:

- Providing an overview of existing synchrotron radiation and neutron facilities, as well as other capabilities as applied to R&D in nanotechnology;
- Identifying the grand challenges of the measurement tasks in characterisation at the nanoscale for the next 5–10 years;
- Defining (a) roadmap(s) for development of the next-generation instrumentation(s) at the major user facilities for characterisation and metrology;
- Identifying short-term and long-term R&D needs for sample environment, optics and detectors;
- Formulating recommendations, priorities and challenges for future research in nanometrology, standardisation and instrumentation;
- Implementation of metrology at basic research as early as necessary to improve the linkage to industrial products;
- Identifying the required developments in theory, modelling, simulation, analysis, high-speed computing, and large-scale data analysis;
- To set-up and approve theoretical models and computing techniques to get insight of details beyond the experimental obser-

TOOL	TASK	APPLICATION AREA	LABORATORY/ PRODUCTION EQUIPMENT
X-ray and neutron reflectometry	Qualification of standard specimen	Layer thickness Surface roughness Interface roughness CD line profiles Quantum dots	Calibration for SPM, SEM
X-ray spectrometry	Measurement of fundamental data for spectroscopy model calculations method development	Elemental composition Chemical state	Spectrometers Model-based quantification software
Focused hard x-ray nanoprobe	Imaging of (irregular) 3-D structures Establish correlations to macroscopic (bulk) properties	(Bulk) compound materials Qualification of standards Nanoparticles	Standards for alternative testing methods based on macroscopic (bulk) properties

Table 6.4.1: Overview of synchrotron radiation and neutron usage.

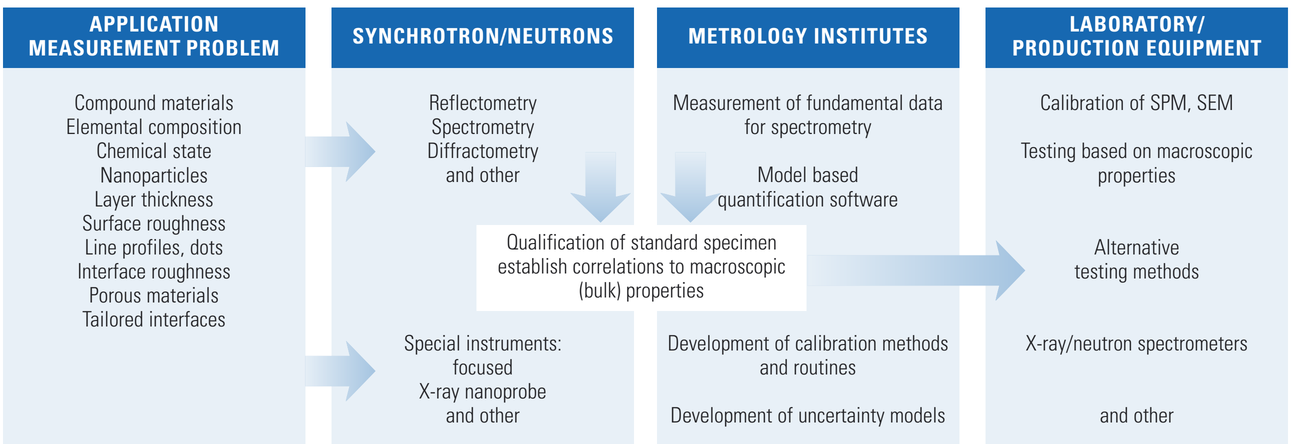

Fig. 6.4.1: Scheme for the development of nanometrology.

vation limit to clarify the limit of uncertainty due to probe – sample interactions (see Fig. 6.4.2);

- To set-up and implement virtual or network based techniques to provide virtual instruments for an improvement of uncertainty calculation, e.g. a virtual scanning probe microscope, for industry;
- To provide standard reference materials to support synchrotron radiation and neutron metrology.

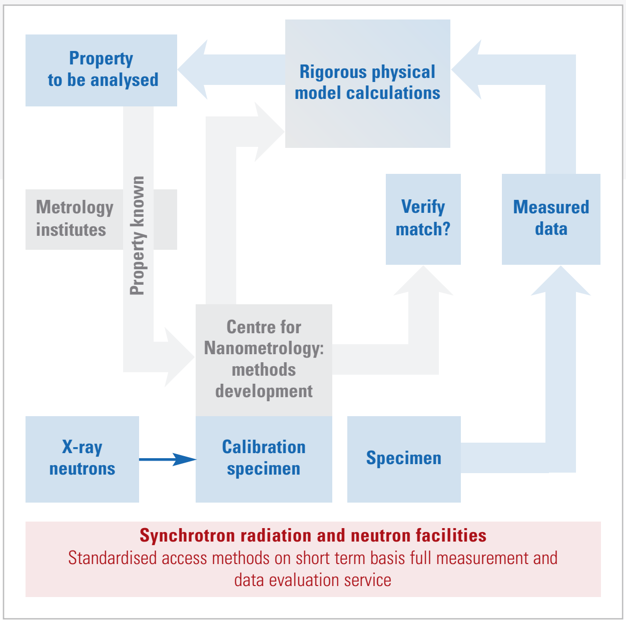

Fig. 6.4.2: Scheme for the development of measurement procedures using synchrotron radiation and neutron probes.

The development of new standard reference materials (SRM) is essential for x-ray and neutron metrology. They are also important for calibrating and assuring the accuracy of measurements, including the correlations between nanoscale structures and their function. These SRMs will assure precision measurement of both bulk nanomaterials and for surface and interface metrology of ultrathin films and layered materials. Among the required SRMs are:

- Nanosized ceramic particles for nanoparticle sizing and aerosol sizing;
- Monodisperse nanoscale SRMs;
- Polydisperse nanoscale SRMs with known size and size distributions;
- Depth profiling standard reference materials for the calibration of XPS and GISAXS are required to assure that surfaces and thin films can be measured with single atom precision.
- In the safety and security arena, ultrafine nanosized particles appear to be more toxic than larger size particles. Knowing the speciation of air-borne heavy-metal particles may facilitate a better understanding of the pathogenic mechanisms of particulate air-pollution. SRMs are needed for carbonaceous soot, sulphates, and nanoscale metal compounds, which dominate the ultrafines in both indoor and outdoor air.

The characterisation of interfaces, inclusions, nanotubes and particles in a matrix etc. will be of increasing importance for nanomaterials characterisation. The only probes providing direct access to such inner properties are TEM, x-rays and neutrons. The corresponding measurement schemes, however, are always based on the measurement of respective x-ray and neutron reflection, transmission, tomography, diffraction, scattering and induced secondary processes such as fluorescence. These measurements are linked to the properties to be measured by the corresponding transport equations. Thus, synchrotron radiation and neutron measurements are highly complex inverse problems. A crucial issue for further development of those methods is therefore a careful evaluation of the corresponding models and numerical algorithms. A scheme for such development is shown below together with a selection of the most prominent synchrotron radiation measurement methods which can be used (see Fig. 6.4.3).

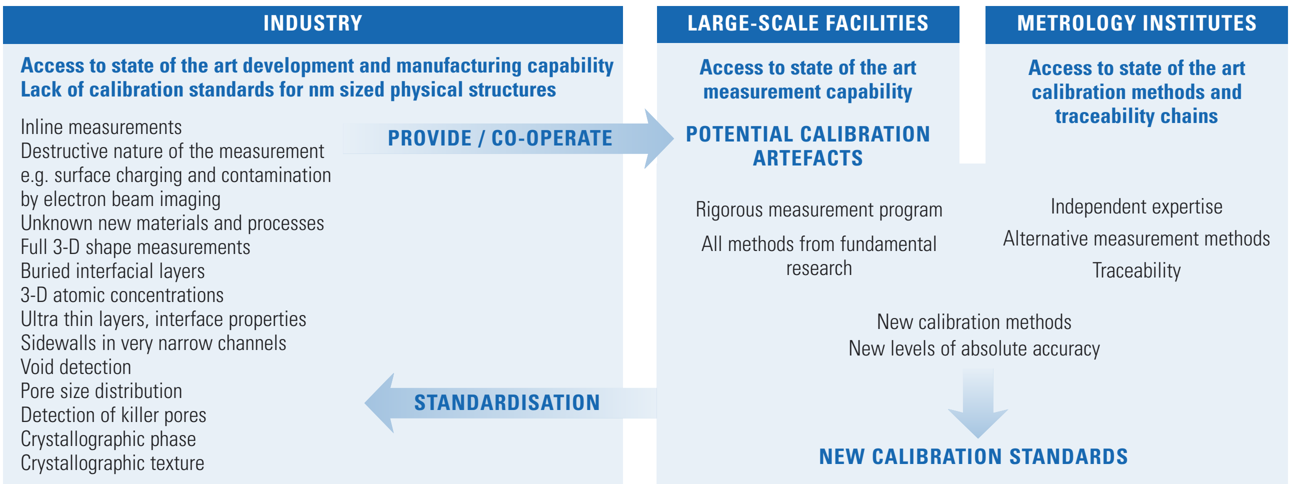

Fig. 6.4.3: Working scheme for the development of standard specimens for nanometrology.

6.5. IMPORTANCE OF NANOMETROLOGY FOR EUROPEAN SOCIETY AND ECONOMY

Nanostructured devices play a key role in industry, (see Chapter 6 of this document of which the semiconductor industry provides the basis for Europe's Information Society industry). Nanometrology is not just a source of jobs and economic growth in its own right – it is crucial to the European economy as a whole, stimulating growth and innovation across industry.

In the USA, NIST has plans for strategic measurement capabilities and activities with an emphasis on cooperative research with the private sector:

- National nanomanufacturing and nanometrology facility;
- Nanomanufacturing research;
- Manufacturing enterprise integration;
- Expanding access to global markets through measurements and standards.

These activities should enable the Advanced Measurement Laboratory (AML) to perform measurements accurately at the scale of individual atoms [H. Semerjian, NIST – Enabling the Future – Innovation, Trade, Safety and Security – and Jobs, NIST Engineering R&D Symposium, April 6, 2005]. This programme will leverage the AML investments and make its benefits immediately accessible to U.S. manufacturing researchers.

6.6. CONCLUSIONS

Nanostructures also enable many new applications. The development and dedicated design of such devices, however, needs exact knowledge of their properties, i.e. metrology. Successful implementation will depend on effective collaboration and cost-sharing between a diversity of national metrology institutes and the European Commission and industry stakeholders. National metrology institutes and universities will play an important role in the development of new metrology tools; all stakeholders should be involved in experimental validation, testing and demonstration for commercial application. Open access technology centres at universities or national metrology institutes should be used to provide expertise and capabilities.

It is essential to define development paths for the critical measurement problems in nanotechnology on the basis of the most advanced present technologies. For each class of measurement problem, the work should be focused on the presently most advanced industrial (scientific) application in the field.

The European Commission, national governments and industry should support nanometrology, instrumentation research and development, as well as standardisation by:

- Defining key areas with the highest direct economical impact: "European technology roadmap for nanotechnology to guide technology developments";
- Developing a multi-agency research programme;
- Developing a strong educational programme; leveraging national metrology institutes that address the development of measurement infrastructure and advanced measuring instrumentation;
- Setting-up European centres of excellence, involving scientists from metrology institutes, basic research, and industry, located at large scientific test facilities which:
  - Identify the opportunities to address measurement problem;
  - Develop prototype measurement facilities;
  - Provide calibrated standards or validated measurements for the European industry;
- Supporting the standardisation process (which is led by industry).

Although nanotechnology represents varied research organisations and industries, if nanotechnology commonalities and focus could be amassed, a consortium-type organisation would greatly foster urgent instrumentation and metrology needs, this organisation acting as the focal point for European nanometrology issues: "GENNESYS European Centre of Excellence in Nanometrology".

This European centre could address the following issues:

- Incentives such as the development of measurement tools as a criterion for promotions and awarding of tenure are currently lacking to encourage scientists in academia to focus on instrument research and development;
- Develop collaborative multi-disciplinary research activities, demonstrating and validating technology;
- The equipment manufacturers who would be interested in development of new equipments are precluded from some of the funding opportunities that could leverage the high cost of instrumentation development;
- Nurturing the creation of a workforce skilled in nanotechnology building the required new suite of instrumentation and metrology tools;
- To guide technology development and assist instrument manufacturers to provide the needed measurement tools with reasonable lead-time;
- Launching an educational programme;
- Leveraging metrology institutes that address the development of measurement infrastructure and advanced measurement instrumentation.

6.7. RECOMMENDATIONS

- **Instrumentation:** Efforts should be made to locate possibilities for instrument builders to establish instrumentation that suits industrial users and ease the transfer of scientific results into industrial production by having access to easy-to-use, fit for purpose and reliable instrumentation.
- **Standardisation:** The existing European committee for standardisation for nanotechnologies (CEN/TC 352) should work closely with the European nanotechnology industry to identify and deliver standards that reflect the needs and priorities of that industry. Consideration should be given to the introduction of new deliver-

ables to meet the needs of industry, which request shorter and shorter time between scientific discoveries and industrial applications.

- **Metrology:** Reference standards as well as traceability to measurements should be developed hand in hand with the GENNESYS scientific roadmaps. Synchrotron radiation and neutron facilities should be used to develop unique reference standards which will revolutionise the way traceability is established between primary standards and the industrial user.

6.8. INSTITUTION OF A EUROPEAN CENTRE FOR NANOMETROLOGY

The establishment of an European meeting point for nanomaterial metrology is essential for the exploitation of this emerging discipline, and to help ensure its successful growth and the promotion of the GENNESYS platform (see Fig. 6.8.1).

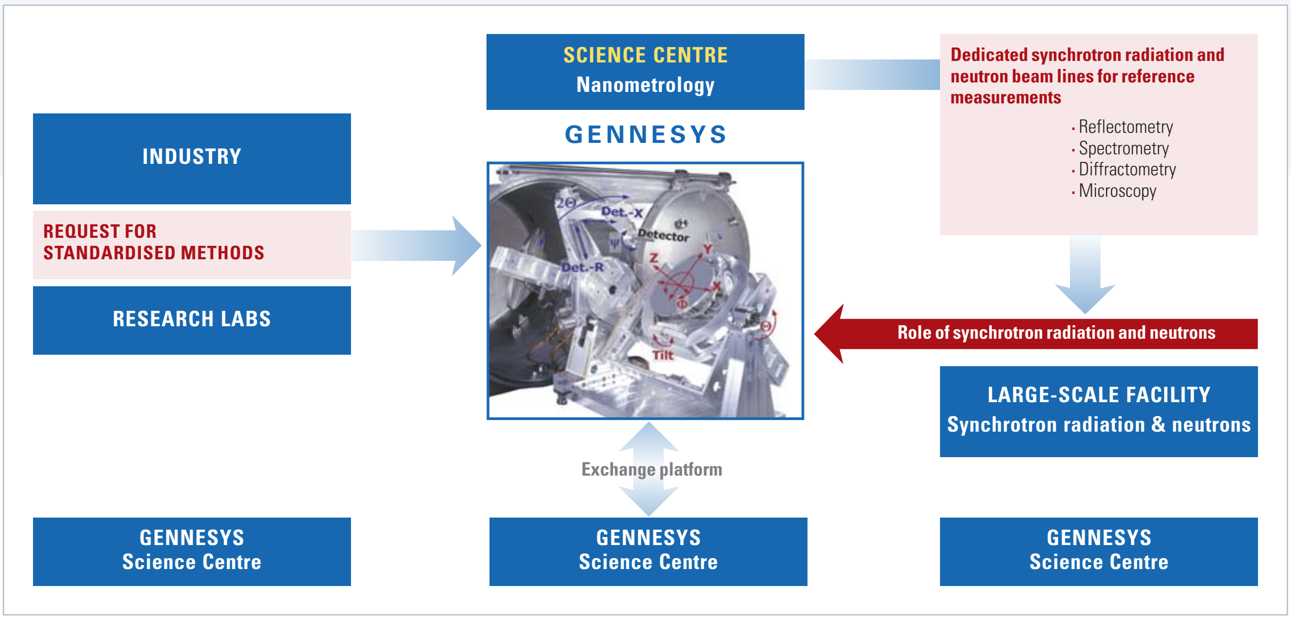

Fig. 6.8.1: Operation of a European Centre of Excellence for Nanometrology.

7. IMPLICATIONS OF GENNESYS FOR INDUSTRY

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7.1. IMPORTANCE OF NANOTECHNOLOGY

The field of nanotechnology is one of the fastest growing and most important scientific developments in the last quarter of a century. European industry has recognised its significance to many industrial sectors and that it will bring extraordinary benefits to our industry, economy and welfare in the next decade. In view of its novelty and complexity, the importance for industry to engage in partnership with the scientific community is obvious, requiring highly skilled workforce and the most advanced test facilities to complement in-house R&D activities.

Extraordinary advances in instrumentation and powerful new experimental tools for research, provided by both national and European synchrotron x-ray and neutron facilities, are opening up the window to gain knowledge on how to control and manipulate atoms individually, observe and simulate collective phenomena on nanometre scale, probe complex material and biological systems. Applications range from nanofabrication of electronic devices to probing the secrets of nanomechanics and nano-bio folding (see Table 7.1.1). The discoveries and innovations bridge length scales from atoms to our everyday experience and will continue to lead to many new and unanticipated developments, as well as products such as light-weight materials, self-cleaning clothing, protective coatings, etc.

The industrial importance attributed to nanotechnology stems from the ability to tailor the functionality of components on the nanoscale and is sketched in Table 7.1.1. These highly complex research and development tasks require effective coordination of the extensive resources available at the national and European level (universities, research institutes, and industry) in order to construct a suitable European infrastructure with coordinated access to versatile analytical tools.

Nanotechnology in industry possesses a distinct cross-technology character; it employs fundamental nanoscale effects absent in the larger bulk for tailoring properties of materials in nearly all material classes to produce improved functionality of devices in various technological fields. This versatile character of nanotechnology further enables application in diverse market sectors and branches of industry (see Fig. 7.1.1). It is furthermore generally acknowledged that the synergetic and convergent development of nanoscience and nanotechnological applications may give rise to unexpected new products.

Information and communication technology	New optoelectronic & molecular electronic devices, new computer concepts (quantum computer); Advanced microelectronic (nanoelectronic) devices; Displays; data storage
Engineering materials	Nanostructured materials: metals, ceramics, intermetallics, nanoparticle-loaded/strengthened polymers (composites), carbon nanotubes as strengthening components
Surface coatings	Surface functionality and improvement, including paints and adhesives
Energy conversion and use	Photovoltaics, thermovoltaics, fuel cells, hydrogen storage materials, batteries/rechargeables, propellants, additives, lubricants
Sensors/actuators	Materials and devices to generate, transduce, receive and transform mechanical, electrical, optical, chemical, and other signals
Catalytic synthesis	Catalysts, photocatalysts, catalyst substrates, nanoreactors, filters, adsorbents, ion exchangers
Health & cosmetics	Diagnostic and therapeutic systems (biochips, contrast agents, drug delivery), improved implants, biological decontamination agents, cosmetics

Table 7.1.1: Examples of nanoscale based new materials and innovative products.

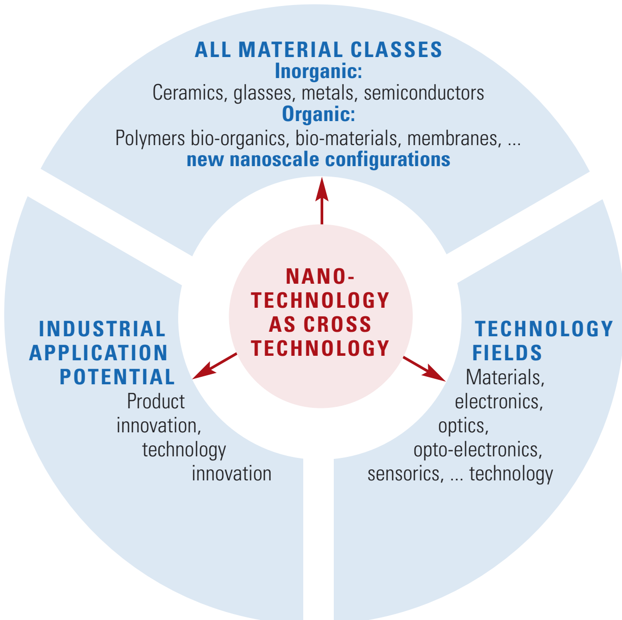


Fig. 7.1.1: Nanotechnology as transsectoral technology influences all important materials classes and technology fields, providing both product and technology innovation.

Nanotechnology is driven by the potential that nanostructured materials or systems have properties which surpass, often by a large margin, those of any existing materials. This translates into cost-savings as well as improvements of performance and functionality and applies to the low-tech branches (construction and textile industries), the so-called core branches of national industries (automotive- and chemical industries) as well as the high-technology industrial sectors (telecommunications, transportation, defence, energy industry, pharmacy, medical engineering and consumer goods). The development of advanced materials that are lighter, stronger, cheaper and more versatile than existing ones will be an important asset provided by nanomaterials discoveries (see Fig. 7.1.2).

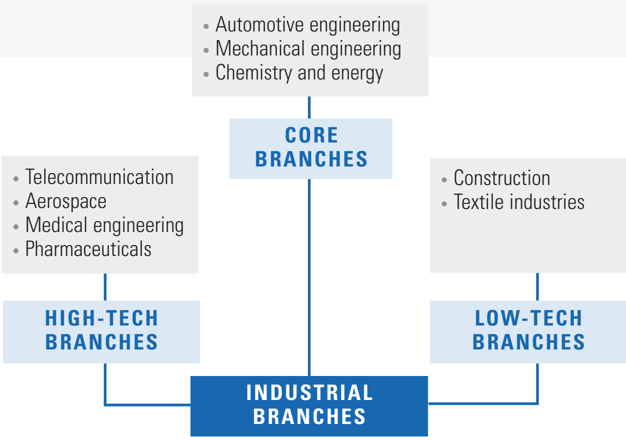


Fig. 7.1.2: Branches with impact of nanotechnology on high-tech, low-tech and core industrial branches.

7.2. NANOTECHNOLOGY FORECASTS

Nanomaterials science and technology is a rapidly maturing field and predicted to become one of the most important key technologies of the 21st century. It will profoundly change major industries and is currently regarded as the greatest challenge to public and industrial research and development (on regional, national, European, and global level) with impact in new and improved nanomaterials and visionary new product concepts. Previous studies[1] of the commercial potentials and the economic advantages predict that nanotechnology would exceed € 800 billion by the end of 2010 in the world economy, i.e. this would become comparable to the present global informatics market.

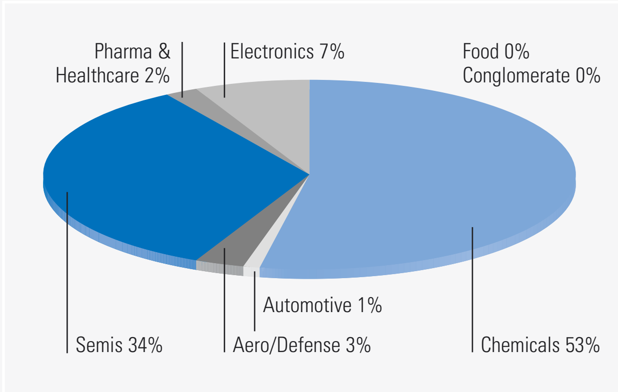


Fig. 7.2.1: The nanotechnology market in 2007.

Fig. 7.2.1, Fig. 7.2.2 and Fig. 7.2.3 give a picture of the expected market developments for prospective technologies in the next decade.

These predictions have stirred intense international competition to secure success in the future nanotechnological markets:

- At present: through technology push, nanotechnologies will become a strategic motor of technological innovation in industry;
- In future: the technological impetus of market pull will increasingly dominate trends for nanotechnology development akin to the development seen in microelectronics in recent years;
- Industrial success strongly depends on efficient science and technology knowledge transfer between research institutions and industry, partly through the success of start-up and spin-off companies, especially in Europe;

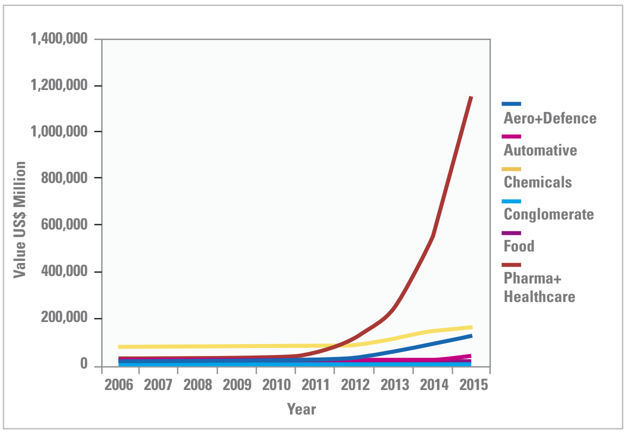


Fig. 7.2.2: Nanotechnology market evolution 2006–2015.

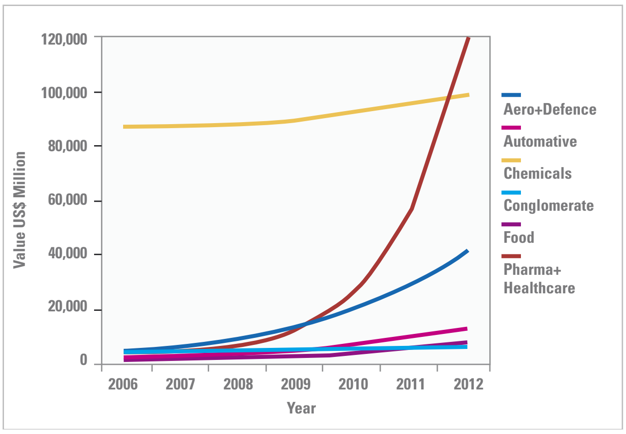


Fig. 7.2.3: Nanotechnology market evolution 2006–2012.

1 The World Nano-Technology Market "An industry Update 2005"

Nanotechnology will revolutionise traditional industries, stimulate development in existing businesses and to create new markets and new industrial spin-offs. It is worth mentioning that, despite the huge variety of products and materials, future needs focus on similar nanobased concepts and technologies (see Fig. 7.2.4).

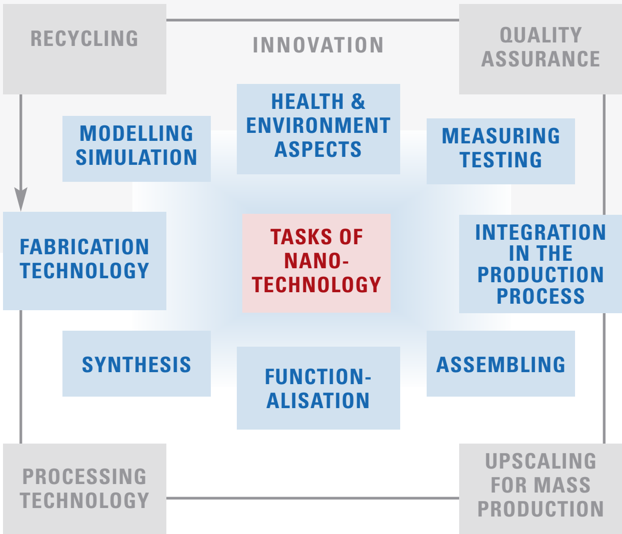


Fig. 7.2.4: Interaction between nanomaterials science, nanotechnology and industrial innovation.

7.3. NEED FOR INDUSTRIAL RESEARCH ON NANOMATERIALS

Challenges for industrial breakthroughs in nanomaterial innovations:

Nanotechnology has fostered the convergence between fundamental and applied research, as well as industrial processing/fabrication and the challenges ahead include:

- *Industrial research:* new methods of synthesis, tailoring of new nanomaterials, functionalisation of nanostructures, chemical and physical surface modification, assembly into systems and integration into devices, material characterisation – nanoanalytics (structure, properties, functionality);
- *Mastering processing and production technology development:* monitoring of basic material physical properties during the development /processing phases in-situ and ex-situ;
- *Up-scaling fabrication and processing techniques:* serial and mass production; quality assurance and control; integration of new nanocomponents in existing production processes;
- *"Certified" nanoscale measurement and testing method development:* industrial application, metrology, standards; cross-sector compatibility;
- *Damage mechanisms during industrial service operation:* in-situ experiments in industrial simulating environments e.g. pressure, mechanical stress, fatigue, corrosive environments, magnetic and/or electric fields;
- *Maintenance, autodiagnostics* and self-healing capabilities;
- *Health & environmental impact:* health monitoring, degradation, recycling, regeneration, waste-management

Need for tools of nanoanalytics and diagnostics for industrial R&D and quality assurance (Fig. 7.3.1)

i) Development of measurement techniques for nanotechnology: new and efficient analytical and characterisation tools are essential for technology innovation on the nanoscale. The property-determining factors of nanomaterials and structures lie outside the range of conventional macroscopic parameters of classical physics. Hence, an adequate experimental acquisition of the real structure and properties of nanostructures and nanomaterials and structures necessitates new definitions of characteristic material and quality parameters, suitable measurement values, and experimental techniques to an extent that has not been developed so far. Development of appropriate measurement technology therefore is of crucial importance to the industrial breakthrough of nanotechnology.

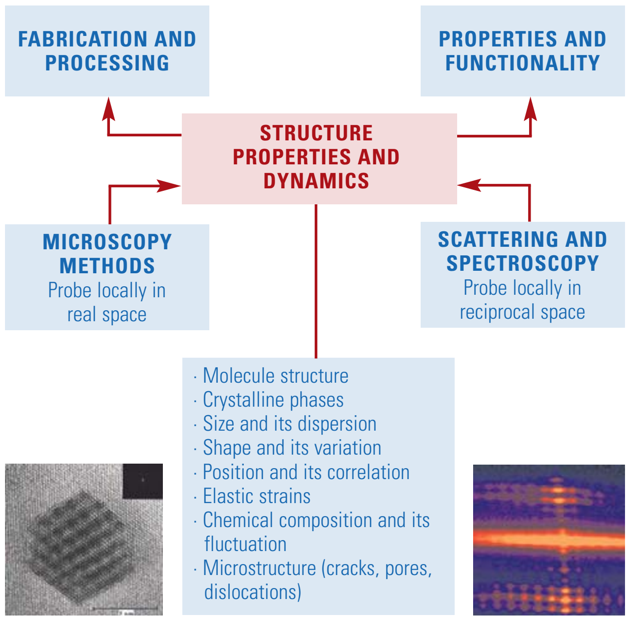


Fig. 7.3.1: Important parameters for the characterisation of nanomaterials and nanostructures.

ii) Failure prevention investigations: The consequences of systematic production failures and failure costs during the development and production phases play a dominant role in the lifetime of components and devices (see Fig. 7.3.2).

New precise and fast analytical measuring techniques and tools for quality assurance in processing and for behaviour in service play an essential role in all stages of product development and reliability. The need for synchrotron radiation and neutron facilities arises from special requirements beyond the capabilities of laboratory equipments, especially high brilliance to investigate small sample volumes and allowing for time-resolved measurements, high resolution in energy, space and angle, tuneable energy and new contrast mechanisms.

Synchrotron radiation and neutron facilities provide powerful non-destructive testing tools best suited:
a) To gain process-understanding, process-modelling and calibration on the laboratory level as a base for optimisation, up-scaling models and process controlling;
b) For in-situ damage and failure analysis, as a base for modelling damage mechanisms, reliability estimations and lifetime predictions;
c) To develop, calibrate or transfer non-destructive measuring techniques for off-line and in-line testing and process control adopted to special needs of nanotechnology

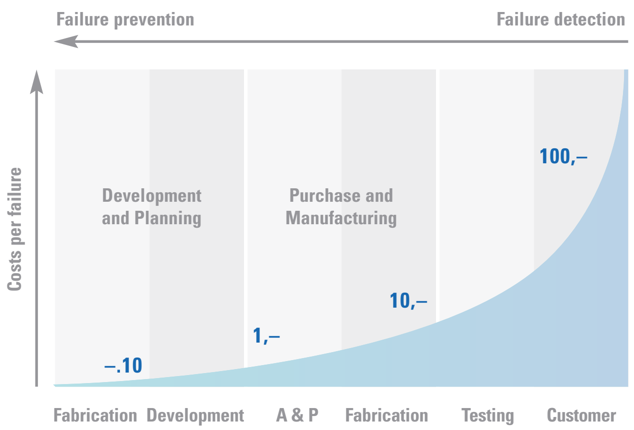


Fig. 7.3.2: Failure costs and "rule of tens".

iii) Risk assessment for health and environment:
Nanotechnology brings about new and specific risk. The increased reactivity of high surface/bulk ratios of nanoparticles implies that risk assessment of bulk materials cannot be readily transferred to nanomaterials. Many of the concerns evolve around free, sometimes toxic, manufactured nanoparticles which can enter organisms in various ways. The implications have not yet been taken into account by health and safety regulators, partly due to the lack of analytical tools allowing detailed characterisation of the life cycle of nanoparticles.

7.4. INDUSTRIAL RESEARCH AT LARGE-SCALE FACILITIES

The nanotechnology scale is not yet fully explored due to lack of efficient/available analytical and characterisation tools, in particular in-situ. However, the novelty and complexity of the technology will catalyse the growing interest in partnership between industry, the scientific community of nanotechnology and the measuring technology and could progressively involve European synchrotron radiation and neutron facilities.

Need for nanomaterial inspection at synchrotron radiation and neutron facilities

- Non-destructive measuring tools of nanoanalytics and materials diagnostics best suited for in-situ detection of structure and property evolution are tightly linked to nanotechnology synthesis, processing, and assembling.
- Optimisation of industrial fabrication processes requires a deep understanding of the physical, chemical and biological principles of synthesis, functionalisation, and assembling processes. That is why a main requirement to synchrotron radiation and neutron facilities considers in-situ techniques allowing to study processes such as deposition of coatings, corrosion etc. under conditions of harsh environment similar to that of industrial processing or device operation.
- Proper length scale, namely from atoms to daily-life scale;
- Excellent penetration into materials, non-destructive;
- In-situ studies (under load, cycling, high P, high T);
- The limitation in flux, brilliance, coherence properties and wavelength range of conventional laboratory light sources and the non-availability of laboratory neutron sources stimulate industry to search for alternatives including the option of using the exceptional potential of synchrotron radiation and neutron facilities.
- Interface laboratories offering support in the access, planning, undertaking and evaluation of experiments at synchrotron radiation and neutron facilities to overcome the hurdles posed by lack of training, expertise and man-power in the private sector.

Industrial barriers to synchrotron radiation and neutron facilities

The selective use of synchrotron radiation and neutron facilities offers clear advantages to industrial research and development. However, industry (or generally speaking the private sector) does not benefit from this opportunity; the use of the synchrotron radiation and neutron facilities is essentially limited to and achieve via universities and/or research institutions on non-confidential advanced or pre-sensitive research topics. Only in exceptional cases does European industry carry out experiments directly related to industrial innovations and process development or production control activities at the synchrotron radiation and neutron facilities. The use of European synchrotron radiation and neutron facilities for industry-driven activities in Europe is low compared to the USA and Japan where most facilities host one or several beam-lines built and operated by companies. Difficulties in integrating large pooled facilities in company's quality management systems are one of the inherent drawbacks.

The lack of uptake of synchrotron radiation and neutron facilities by industry can be summarised as:

- Synchrotron radiation and neutron facilities are biased, sometimes explicitly in their statutes, to public basic research, rather than applied research resulting in limited focus and scope of provided service, inflexible access procedures, lack of support for non-expert users;
- Lack of communication between the research community, the facilities and industry; competitive behaviour between synchrotron radiation and neutron communities;

- Lack of information, education about available techniques;
- Lack of standardisation and certified repeatability of experiments.

There is a striking exception to the above-described mediocre situation concerning the industrial access at synchrotron radiation and neutron facilities: the "industrial application of commercial services" in pharmaceutical macro-molecular-crystallography. It represents a model of the successful use of large-scale facilities by industrialists. The reasons for success encompass the whole organisation of science and technology, and include the following factors:

- Experimental equipment and protocols are developed and optimised for both academic and industrial interests: robust standard methods, reliable instrumentation, a high level of automation of the measuring procedures, high sample throughout;
- Data collection processes are further standardised and automated and entered the data processing phase;
- Pharmaceutical preparative and post-experiment analysis laboratories are available at site;
- Dedicated services are offered by the synchrotron radiation and neutron facilities: staff and equipment;
- High standard support laboratories on site.

In summary, the collaboration with the pharmaceutical industry has resulted in a full integration of the synthesis and analytical laboratories within the infrastructure of the synchrotron radiation and neutron facilities.

- High investment and operation costs: use of beam time and personnel;
- Long delays for access to the beam lines;
- Limited industrial interest: lack of synchrotron radiation and neutron facilities staff motivation and skills concerning industrial needs;
- Lack of adapted equipment or ready-to-use techniques for industrial needs;
- Lack of industry-friendly environment and mentality/spirit at large-scale facilities;
- Almost no knowledge in industry about synchrotron and neutron scattering;
- Confidentiality problems;
- Facilities do not deliver the level of service necessary for industrial purposes;
- Missing long-term research strategy by industry (industrial use of synchrotron radiation and neutron facilities needs longer timescales than just using table-top instrumentation).

Recommendations – challenges and breakthroughs

European industry recognises the fast growing scientific developments in nanotechnology and its future significance to many industrial sectors. In order to overcome the above mentioned barriers, it is recommended to foster the collaboration between industry and synchrotron radiation and neutron facilities which would be beneficial to all partners and offer new challenges for the synchrotron radiation and neutron facilities while making them global leaders in lucrative nanomaterial research. If integrated into technological networks of competence, synchrotron radiation and neutron facilities could reach out to novel user groups, provide valuable measuring services beyond the capabilities of laboratory and table-top instrumentation and thus prove suitable for systematic technology optimisations. Academic industrial collaboration would lead to the creation of strong links between large scientific facilities and the European innovative industry. This is an opportunity and beneficial to both as well as for the wider European community.

The challenges for synchrotron radiation and neutron facilities are to satisfy the industrial needs as regards confidentiality, quality, repeatability, efficiency and costs. Therefore, the performance parameters of facility instrumentation should be adjusted to include applied sciences and be industry-friendly as preconditions for breakthroughs in product innovations which are related to clear customer benefits (see Fig. 7.4.1). A key role for successful exploitation of these facilities are so-called interface laboratories where resident scientists with strong industrial expertise can act as contact points, liaise with industrial collaborators and local scientists (e.g. beam line scientists), and bridge the mentality gap.

Industrial quality assurance in nanotechnology has to meet the same requirements as other research and development sectors: reliability of the measuring technique; unification of data evaluation; cross-compatibility; clarity of interpretation, ease of use. Consequently, instrumentation does not necessarily require highest precision, but the highest efficiency, reliable quality, and justified costs. "Workhorse" instrumentation does not mean lower quality, but certainly differently optimised equipment, with a high degree of automation, flexibility of access, high sample throughput including data analysis, and guaranteed standards. Additionally, participation of industrialists in the synchrotron radiation and neutron facility decision-making processes should be encouraged.

Additional competitive advantages for neutron and synchrotron sources could come from specific services such as: validation; metrology; tracing; standardisation up to certification of methods; accreditation of laboratories; education and training.

Scientific and technical support issues

Synchrotron radiation and neutron facilities should provide an efficient and reliable service to the industrial scientific guests:

- Provide all necessary scientific support related to special facility techniques or academic knowledge;
- Assist in designing experimental set-ups and data analysis;
- Work out procedures for "full service" i.e. from problem specification to data collection, analysis and interpretation.

CHALLENGES
High quality, high efficiency, low costs

Automation of measurement and evaluation
Unique interpretation, validation
In-situ measuring techniques
Combination of measuring techniques
Metrology, calibration for laboratory methods
Table-top synchrotron
On-site nanotech infrastructure, networking

Performance parameters of large-scale facilities as standard measuring technology

BREAKTHROUGH
Customer benefit

High throughput screening
Reliability standards
Optimisation of fabrication and processing technologies
Quantitative structure property relation
Process integrated non-destructive testing
(on-line quality insurance)
Customer-adapted, one-stop shop

Fig. 7.4.1: Overview of technological tasks – Challenges for large-scale facilities responding to industrial-customer benefits.

Meeting the requirements of the following aspects would result in exciting challenges for the nanomaterials industry in Europe:

- Economic aspects;
- Logistic aspects;
- Networking and partnership alliances;
- Technological factors.

However, it should also be recognised that these criteria form the preconditions to reach a breakthrough for the use of synchrotron and neutron facilities in industrial nanomaterials industry. Logistic aspects also consider accessibility, the geographic distance and technological environment of the facility.

7.5. SYNCHROTRON RADIATION AND NEUTRON TECHNIQUES

A large range of measuring problems remains in nanomaterials science, where conventional laboratory methods fail or reach their limits. The unique capabilities of neutron- and synchrotron measuring techniques may well gain scientific insights and have valuable technological impacts if they provide reliable problem solutions beyond the limits of laboratory techniques.

In this context we refer mainly to established synchrotron and neutron methods, which have already crossed over from curiosity-driven research at the facilities to reliable measuring technology, which is well-calibrated and includes the potential for metrology and successful certification (see Table 7.5.1).

Synchrotron and neutron methods for material diagnostics and non-destructive testing, especially strain/stress analysis, computed tomography, powder diffraction, element analysis, complex analytical services by inelastic spectroscopy and small-angle scattering could have the potential to complemement industrial laboratory ex-situ and in-situ measuring techniques of nanoanalytics and material characterisation. Their use may be rewarding during the whole material life cycle: from the development phase of nanomaterials and nanodevices to non-destructive testing and quality assurance (see Fig. 7.5.1).

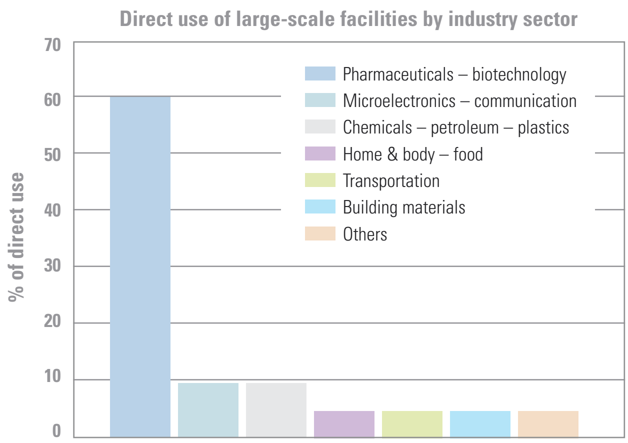


Fig. 7.5.1: The sectors of industry involved in direct use of European large-scale facilities are: (about 3% overall).

Potential industrial use of synchrotron and neutron facilities will be based on:

- "Workhorse" facilities for reliable analytical services to characterise structure, properties, and fabrication processes;
- Services for quality assurance, including material characterisation, non-destructive testing of devices in harsh environment or under industrial operation conditions, failure analysis, reliability and life time estimation, calibration of laboratory methods;
- Services in prototyping and micro- and nanopatterning, (especially of non-silicon materials and based on deep x-ray lithography). Here, the main challenges are related to: a) Up-scaling of the patterning processes on large areas, b) reliability, c) reduction of costs;
- Cutting-edge installations for breakthrough research of new measuring techniques for nanoscale properties;
- The conversion of synchrotron techniques to table-top equipment.

Fig. 7.5.2 shows the potential and the diversity of the industrial issues that can be approached using radiation-based analytical and characterisation techniques. The nanolabs at the large-scale facilities GENNESYS technology centres (see section 7.6.5) allow to measure the evolution of nanostructure and properties in-situ during fabrication and processing by simultaneous use of synchrotron and/or neutron methods and complementary chemical/physical or analytical techniques.

Activity	Technique	Synchrotron radiation	Neutrons
Protein structure determination	Diffraction	X	
Characterisation of drug polymorphism	Diffraction	X	
Stress-strain analysis for metallurgy and plasturgy	Diffraction	X	X
Characterisation of semiconductor devices	Diffraction	X	
Relation mechanical properties – molecular structure of fibres	Diffraction	X	
Assessment of the effectiveness and safety of cosmetic products	Diffraction	X	
Stability and ageing of foodstuffs	Scattering	X	X
Characterisation of colloids, emulsions, gels etc.	Scattering	X	X
Follow-up of cement setting, clinkerisation	Diffraction	X	X
Characterisation of the molecular and microstructures of plastics	Diffraction	X	X
Understanding catalytic reactions for new catalyst development	Absorption spectroscopy	X	
Characterisation of the oxidation state for environment	Absorption spectroscopy	X	
Chemical characterisation of surface treatments and thin layers	Absorption spectroscopy	X	
Research and development of new fine chemicals	Absorption spectroscopy	X	
Detection of trace elements	X-ray fluorescence	X	
Distribution of elements in biomaterials	X-ray fluorescence	X	
Organic product identification and diffusion of product	IR-microscopy	X	
Visualisation of magnetic domains	PEEM	X	
Detection of microcracks	Tomography	X	
Analysis of the porosity of rocks and building materials	Tomography	X	X
3-D imaging of composite materials	Tomography	X	X
Detection of defects in large pieces	Neutrography		X
Lithography for microelectronics	UV-insolation	X	
Microfabrication	LIGA process	X	

Table 7.5.1: The main activities related to direct use of European large-scale facilities by industry.

As nanotechnology most often deals with small objects or composite objects, the analyses have to be carried out at the micrometer-, submicrometre- or nanoscale in mapping mode. In addition, transformations may occur at timescales as small as micro- or nanosecond, it is therefore of prime importance to follow as much as possible the transformation in real-time. Powerful non-conventional radiation sources are then necessary to match this spatial and temporal resolution, i.e. synchrotron and high flux neutron sources.

Other goals for large-scale facilities commitments in nanotechnology should be the transfer of know-how in measuring techniques and instrumentation to industry. Already today, successful industrial collaborations and outsourcings deal with the transfer of technologies and know-how, concerning x-ray optics and detectors, components and products developed at large-scale facilities. Industrial quality assurance departments ask for process-integrated non-destructive testing techniques, health monitoring, and process control, tasks which are difficult for large-scale facilities to solve. Synchrotron facilities may contribute to a major breakthrough in this field by transferring suitable methods to optimised laboratory solutions that may be integrated in industrial labs or even serve as inspection tools within the production lines. For these reasons, it is recommended to analyse the potential of miniaturised table-top synchrotron radiation machines.

Stimulated by the worldwide transition from film to digital imaging detectors, the market of x-ray inspection methods shows the largest growth rates on the global NDT market with increasing potential. Both the NDT market and the market of x-ray-based nanoanalytics would strongly benefit from table-top synchrotron sources, since they would offer to employ various methods in industry, which are so far restricted to large-scale facilities which are mostly oriented towards fundamental research.

Table 7.5.2 shows potential applications of radiation-based analytical techniques to study multiple phenomena in a wide range of industrial branches for new discoveries and product innovation.

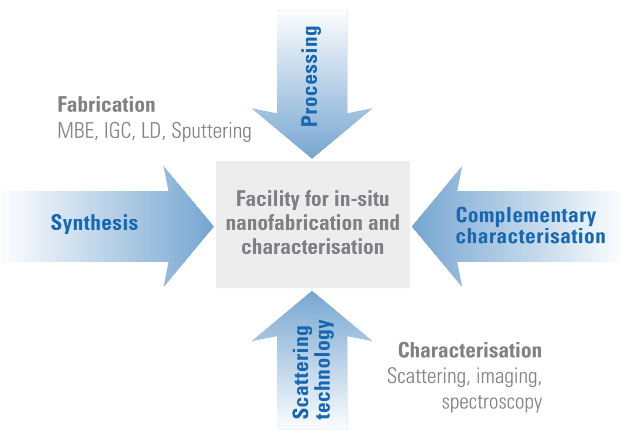
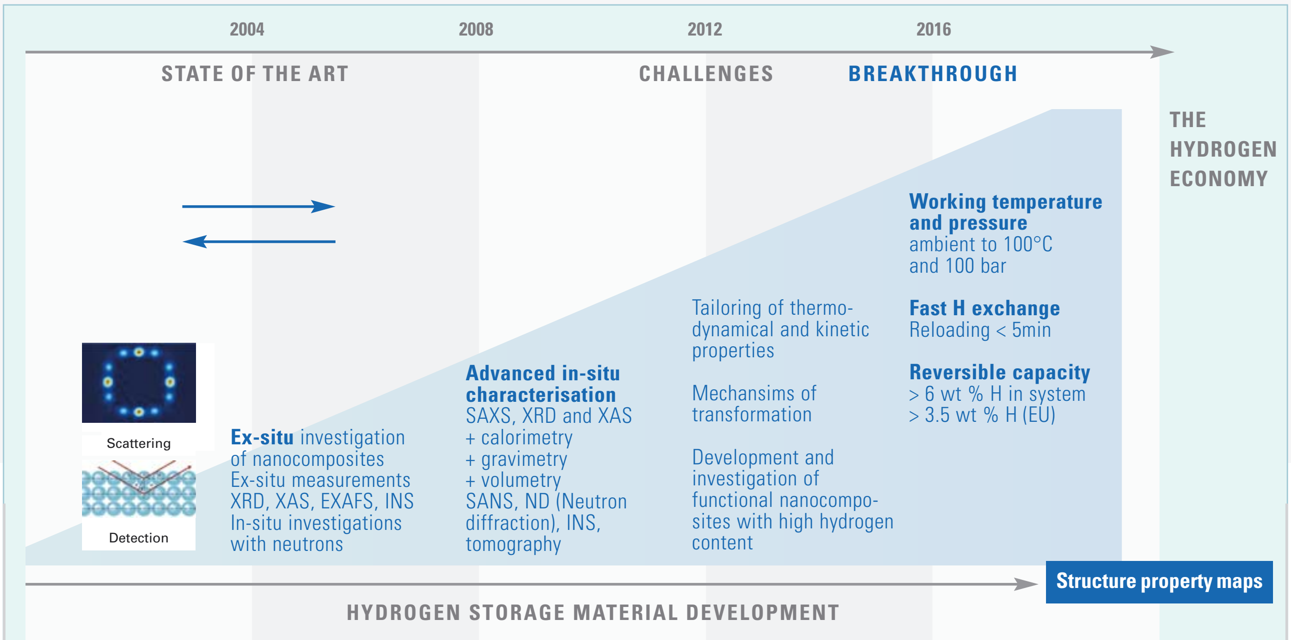


Fig. 7.5.2: Schematic illustration of the potential and diversity of individual issues handled at large-scale facilities.

TECHNIQUE / SECTOR	DIFFRACTION/SCATTERING	SPECTROSCOPY	RADIOGRAPHY & IMAGING
	Diffraction Small-angle scattering Biocrystallography Powder diffraction Laue diffraction	EXAFS XANES Photoemission INS (Inelastic neutron scattering)	X-ray fluorescence XANES FT-IR Tomography Radiography PEEM
ELECTRONICS	Stress in sub-μm lines in chips Detection of point defects	Surface characterisation Local chemical environment	Magnetic layers in lecture head Detection of voids and failures
METALLURGY	Local stress gradient Nanomorphology Nanoclusters in alloys	Surface oxidation	Micro- and nanostructure Voids and microcracks
AERONAUTICS/CAR	Stress in turbine blades Lighter materials Welding of aluminium		Micro- and nanostructure Micro-defects Radiation-resistant electronics
GLASS/CERAMICS	Local crystalline ordering	Local nanostructure	Nano- and micromorphology defects
ENERGY	Phase identification Corrosion processes	Ageing processes Reactivity	Distribution of defects Processes in fuel cells
BUILDING MATERIALS	Phase identification Setting of cements and concretes Nano-organisation	Ageing	Micromorphology Inclusions
PETROLEUM MINING	Nanoinclusions in minerals Solid deposits in oil Colloidal particles	Identification of minerals	Sub-μm porosity and inclusions
PETROCHEMISTRY	Chemical transformation Crystallisation	Nanoaggregates for catalysis	
PLASTICS	Nanomorphology Skin-core structures Nanofibrils in fibres	Morphology of multiphase materials Drug delivery	Micromorphology Defects Distribution of charges
FINE CHEMICALS	Phase identification Nanoreactors	Nanochemistry	
COSMETICS/ HOME PRODUCTS	Nanomorphology of micelles, gels, emulsions Assessment of the effects in tissues at the molecular level		Micromorphology Penetration of cosmetics in tissues
WOOD/PULP	Quality and orientation of fibrils	Speciation during bleaching	Distribution of chemical elements Micromorphology
FOOD	Stability and ageing of colloidal foodstuffs	Free radicals	Micromorphology of emulsions, fats etc.
PHARMACEUTICALS BIOTECHNOLOGIES	Protein-drug interaction Crystalline polymorphism Colloids for drug delivery	Drug after delivery	Micromorphology in drugs and tissues Distribution of chemical elements
DEFENSE	Nanophase characterisation Chips for sensors	Speciation Reactivity	Microcracks Radiation-resistant electronics
ENVIRONMENT/ HEALTH BIOMEDICAL	Nanoparticles identification	Speciation for remediation	Sub-mm morphology Radiological diagnosis Distribution of chemical elements

Table 7.5.2: Overview of radiation-based analytical and characterisation techniques for the nanomaterial industry.



HYDROGEN STORAGE: AN IDEAL MODEL FOR A LARGE-SCALE FACILITY LABORATORY

Nanotechnology approaches the aim of making tailor-made developments for nanomaterials for hydrogen storage.

Crucial challenges for research and development concern:
Development of appropriate functional nanocomposites with constituents of H-rich carriers (e.g. hydrides) and nanoscale dopants;

- Optimisation of the mechanisms of transformation;
- Tailoring of the thermodynamical and kinetic properties.

Technological questions concern:

- Up-scaling of nanomaterial synthesis;
- Mechanical alloying.

Crucial challenges for research and development concern the complete hydrogen economy cycle:

- Production
- Storage
- Transport
- Consumption
- Recycling

Hydrogen storage is one of the key issues to be solved for a breakthrough of hydrogen technology in the energy economy. Various ways of storing hydrogen for fuel cell-driven applications, conventional storage systems based on liquefied and pressurised hydrogen, exhibit principal drawbacks. A practical solution would be storage material that can readily take up and release large amounts of hydrogen. Target properties of a hydrogen storage material comprise the hydrogen content, the thermodynamic properties, and the kinetics of hydrogen exchange. According to car manufacturers, more than 6 wt% of reversible hydrogen capacity should be contained in such a system, including tank and valves. The exchange time for reloading should not exceed 5 minutes. Thermal properties of the material have to match the operation conditions of the fuel cell, which means that the temperature necessary to release the hydrogen from the store should not exceed the temperature and pressure of the exhaust gas of the fuel cell (ambient to 100° C, 100 bar).

Nanotechnology approaches aim at making tailor-made developments for hydrogen storage materials. Crucial challenges for research and development are the development of appropriate functional nanocomposites with H-rich carriers (e.g. hydrides) and nanoscale dopants, the optimisation of the mechanisms of transformation, and tailoring the thermodynamical and kinetic properties. Technological aspects concern the up-scaling of synthesis and mechanical alloying. Synchrotron and neutron technology has been shown to be an efficient tool in determining the local structure of nanocomposites. A requirement for large-scale facilities will be the supply of in-situ measurement techniques which combine the following technologies: EXAFS, SAXS, XRD, ND, N-radiography, and SANS with calorimetry, volumetry, and gravimetry. Such advanced measuring stations would strongly contribute to complying with the roadmap for hydrogen storage materials. Due to the privileged contrast of neutrons with hydrogen, neutrons are particularly well-suited to study hydrogen-related problems.

Fig. 7.5.3: Hydrogen storage roadmap.

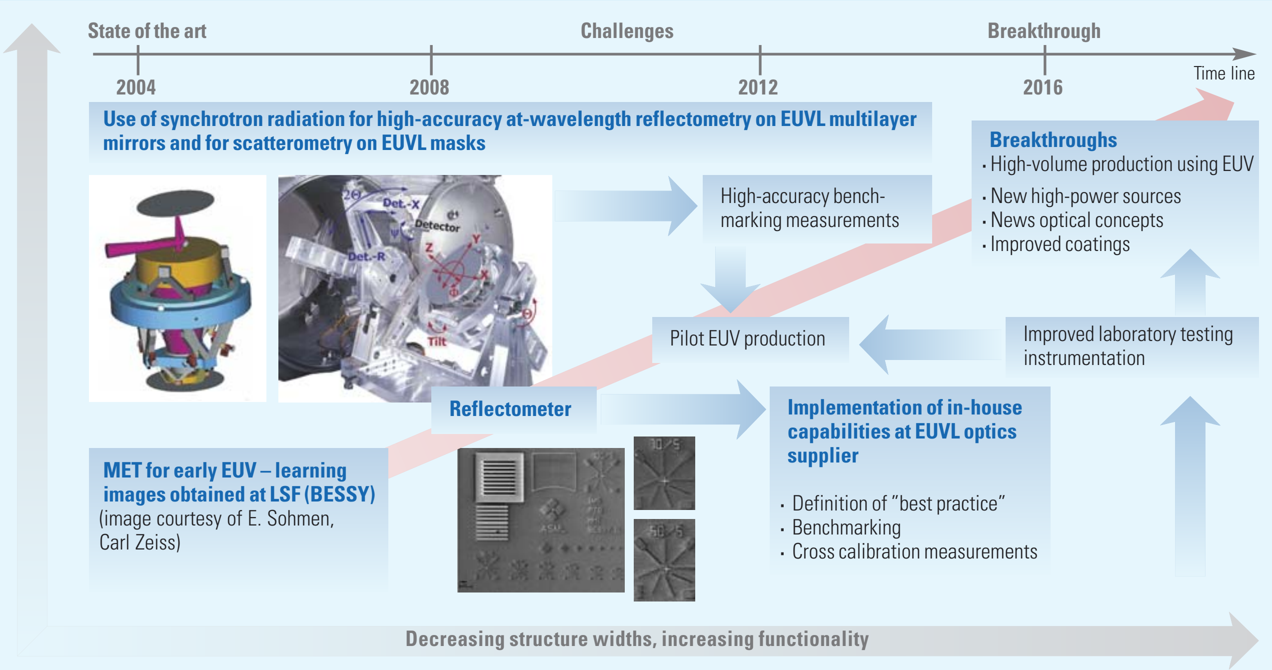


Fig. 7.5.4: The main enabler for the development of the semiconductor industry towards ever new and broader applications in all fields of technology is the continuous shrinkage of the structure sizes. More than 20 years ago, first attempts towards the development of EUVL projection optics were undertaken at governmental and scientific large-scale facilities (LSF) in order to overcome the intrinsic resolution limits of optical lithography. This early development was a precondition to prepare the technology for production readiness around 2011, when DUV lithography will reach the resolution limit for single patterning of dense structures. The panel above highlights the role of the large-scale facilities for the technology development.

Other goals for large-scale facilities commitments in nanotechnology should be the transfer of know-how in measuring techniques and instrumentation to industry. Already today, successful industrial collaborations and outsourcings deal with the transfer of technologies and know-how, concerning x-ray optics and detectors, components and products developed at large-scale facilities (Fig. 7.5.4). Industrial quality assurance departments ask for process-integrated non-destructive testing techniques, health monitoring, and process control, tasks difficult to be solved by large-scale facilities. Synchrotron facilities may contribute to a major breakthrough in this field by transferring suitable methods to optimised laboratory solutions that may be integrated in industrial labs or even serve as inspection tools within the production lines. For these reasons it is recommended to focus attention also to the development on miniaturised, so called table-top synchrotron radiation machines.

7.6. GENNESYS – INDUSTRY PARTNERSHIP: "EUROPEAN TECHNOLOGY CENTRES"

Nanotechnology and new radiation sources offer unique and timely opportunities for the development of collaborative research infrastructures at or in the vicinity of European "large-scale facility" research centres: novel instrumentation, beam lines as well as support and interface laboratories which should be taken care of. The integrative aspects of "industry – large-scale facilities" collaboration will extend to all aspects of facility access and experimental service needs. These elements are of vital importance for the cross-fertilisation of discoveries and the stepping up of technological innovations in the nanoindustry landscape in Europe.

GENNESYS – Industry mission

The vision of the GENNESYS industry initiative is to utilise the fundamental capabilities of large-scale neutron and synchrotron facilities for nanoscience and -technology in both applied pre-competitive and industrial research and development. Large-scale facility technology offers unique analytic solutions for nanoscience and nanotechnology and therefore will enable new scientific insights and breakthroughs in future applications.

The mission of the GENNESYS initiative is to act as a catalyst bridging the gap and building up a European platform for integration of the scientific and technological potentials of nanotechnology and large-scale facilities in a way that allows efficient technology transfer and measuring service for industry. GENNESYS should be a driving force to promote the industrial interest at the large-scale facility management and for adapting, developing and opening the neutron and synchrotron research infrastructures to the "nanomaterials" industry.

The major targets of the GENNESYS-Industry platform should be:

- Catalyse the industrial interest at the large test facility management;
- Promote the adaption of operation and instrumentation of large-scale facilities for industrial purposes;
- Assure a worldwide competitiveness position of the European companies;
- Initiate and support installation of auxiliary laboratories on the site of large-scale facilities dedicated to use by industry, and tailored to their purposes.
- Adapt, develop and open the neutron and synchrotron research infrastructures to the nanomaterials industry;
- Train, promote and advise the private sector, while getting involved with accreditation authorities and industry-wide standardisation efforts;
- Coordinate the relations between the European Commission, industry, funding agencies and large-scale facilities dedicated to nanotechnology;
- Study and assure the implementation of long-term needs for collaborative or proprietory research at large-scale facilities and the coordination with EU directives;
- Explore, define and follow-up of EC actions for launching industry-oriented centres and supporting interface structures between facilities and nanoindustry.

Need for partnerships: university – private sector – radiation facilities

The success of future technology strategies lies on the shoulders of a skilled workforce. To this end, academic – private sector partnerships are of utmost importance:

- Nanomaterials science finds itself close to industry where:
  - The concept of "strategic intent" is applicable to research;
  - The interaction with the science community is vital for the development of the nanofield and its economic impact.
- Continued progress depends on establishing effective partnerships:
  - Across disciplines;
  - Between universities, research laboratories, large-scale test facilities and industry.

Partnership objective: to explore the advantages of "Applied/Industrial Research Networks" and "GENNESYS Technology Centres" as strategic alliances: industrial groupings and research laboratories at large-scale facility sites;

They should operate at the frontier of science in a strategic context:

- Developing broad new understanding to advance both science and technology;
- Making profound contributions with impacts far beyond their corporate borders.

Their role would be to:

- Optimise the use of infrastructure and facilities;
- Enable cross-disciplinary research;
- Improve university, research laboratory and large-scale test facilities' appreciation for industry priorities and needs;
- Share the risks and returns of long-term research;
- Assemble teams that can emulate the fertile research environment of the industrial research laboratories.

Within these partnerships, industry must continue to play a significant role in supporting fundamental research, such that a vision is provided connecting research to the technological applications.

The science–industry–facility partnership model is very promising; it could be a new mechanism for science- and technology transfer into industry and would be successful in developing new nanomaterials science and technology.

Needs for adapting equipment, scientific culture, and access modes at large-scale facilities

In most cases, large-scale test facilities have so far been implemented and operated mainly with the mission of fundamental research and development for the public. The attempts now are to operate successfully large-scale facilities using "partially" market-driven economic concepts.

So far, the few attempts to operate large-scale facilities based on primarily market-driven economic concepts have not been successful. High investment and operation costs still make operational "models based on full return" of investment by acquisition on the free market difficult to realise. The public assignment should be maintained and emphasised for matters related to applied and engineering research. Ways have to be discovered to invent operational schemes based on suitable return models for investment, in order to assure success in the European nanoindustry and nanomaterials markets. Equally, fundamental obstacles such as statutes imposed during the establishment of institutes and which limit industrially relevant research, need to be amended.

The future mission of the large-scale test facilities should be threefold:

- To maintain the public assignment;
- To assure excellent science;
- To put emphasis on applied and engineering research, including direct measuring service for industry.

Management instruments

Professional strategic orientation needs to know the large-scale facilities' interests and commitments in the industrial and public nanotechnology research. Essential points will be the combination of a realistic market strategy with coordinated internal services in order to meet the market-derived requirements of quality, costs, and service.

Corporate identity

Successful impact of the large test facilities nanotechnology activities on industry needs the build-up of a management and institute culture which adjusts internal performance criteria of large test facility instrumentation and staff in accordance with the industrial mission. A science policy needs to be developed which balances fundamental and applied research.

Need for European networking with the large-scale facilities

"GENNESYS" should provide a way to bridge the gaps between large-scale facilities and nanomaterials technology in applied science and industrial research.

Networking between scientific- and industrial research laboratories with large-scale test facilities will be a crucial point to reach an optimum synergy and maximum outputs in nanomaterials science, nanotechnology and nanomaterials markets perspectives. The main role of the networks is to create beneficial and efficient scientific and technological infrastructures necessary to allow smooth operation of the partnerships and the "GENNESYS Technology Centres". Fig. 7.6.1 schematically represents four fundamental types of strategic alliances between the scientific, technological, and industrial communities and the large-scale facilities:

1. Promotion of networking of large test facilities with nanoscience and -technology institutes:

- To build up complementary "nanomaterials" research laboratories on site, at the facilities, which provide complementary infrastructure for nanotechnology (in-situ fabrication and measuring techniques);
- Large-scale test facilities should organise full measuring services for the nanotechnology centres, which should focus efforts on running the fabrication and processing laboratories and techniques;
- Technological relevance should be a second decisive criterion, alongside scientific excellence, for allocating beam time, realised by short-term peer reviewing;
- European industry should be allowed to use the complete infrastructure as a scientific foundry service.

2. Promotion of networking with applied – science institutes/measuring – equipment institutes:

- Industry's needs are not just for beam time, but rather for complete solutions. Requirements for competence within the large test facilities with respect to industrial access, internal project management, professional customers service, the education of interdisciplinary skilled staff, and the implementation of instrumentation, all matching the needs of industrialists, will usually exceed the presently available experience of large-scale facilities.
- The organisation must fit the needs of the nanomaterials scientists with respect to analytics, non-destructive testing, in-situ measuring techniques, etc;
- Large-scale facilities (synchrotron and neutron) could act as experts of beam line construction able to implement synchrotron instrumentation, but should follow clear specifications of the nanomaterials and applied research institutes;
- Performance criteria of applied research and development, such as technological relevance and market relevance should be added to the decision catalogue for acceptance of non-proprietary research proposals.
- Regular long-term supply of beam time and high-quality user support must be ensured.
- Consider the creation of consortia of applied science laboratories: that can be done by promoting the installation of visitor groups of applied science institutes as competence and service centres. Within a partnership, the large-scale facility operates the beam lines, the visitor groups operate the applied measuring stations and integrate them into their portfolio of their home-lab measuring and testing service.

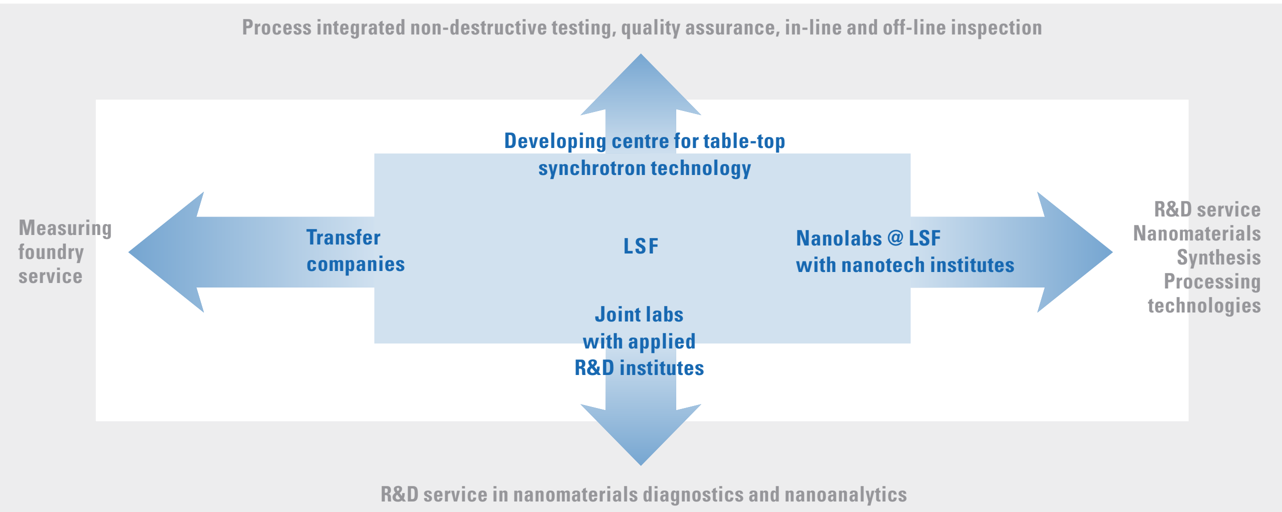


Fig. 7.6.1: Strategic alliances with large-scale facilities.

- Dedicated measuring stations should be fully integrated in the quality management systems of the applied research institutes.

So, the network will supply complete research and technology services for problem solutions covering specification, combination of different necessary techniques, evaluation, interpretation, and validation, all the time keeping industrial interests in mind.

3. Promotion of networking with public research institutions and industrial providers developing synchrotron instrumentation and laboratory x-ray instrumentation (for in-line x-ray inspection, and x-ray analytics):
- Transportable and decentralised, but highly brilliant x-ray sources could bring an enormous breakthrough for such synchrotron techniques especially for industry;
- Time management, full accessibility and quality assurance are essential parts of the protected core know-how. Especially quality assurance in production could profit from measuring techniques suitable for on-line and in-line process control;
- Technical solutions that combine techniques of conventional synchrotron storage rings and those of conventional tubes seem to be promising solutions and close at hand; large test facilities should actively take part in such developments;
- The task of adapting synchrotron methods to industrial nanotechnology and the respective beam line instrumentation to compact laboratory conditions and industrial needs will require collaboration of large-scale facilities with industrial equipment developers;
- The innovation of small "pocket" synchrotron radiation and neutron sources for the materials diagnostics and non-destructive testing and nanoanalytics markets, so-called table-top synchrotrons needs priority development (see Annex I to Chapter 7);
- Transportable and decentralised, but highly brilliant x-ray sources could bring an enormous benefit for such synchrotron radiation techniques especially for industry;
- Since table-top solutions are already a field of strong competition with Japanese and US research institutes and companies, GENNESYS should promote pre-competition development in its funding policy (see Annex I to Chapter 7);
- Laser-based table-top free electron lasers – technical solutions.

4. Promotion of networking to the generation of satellite labs and European transfer centres with start-up funding:
- Consistent transfer between large-scale facility techniques and similar laboratory techniques will be crucial to a sustainable impact of large-scale facilities. It is reasonable to consider implementation of virtual development centres working as a European platform for the transfer of large-scale facility-technology to the modernisation of industrial laboratory equipments.
- A European X-ray and Neutron Technology Development Centre in the form of a European applied research institute could be a catalyst on such a way, working based on a European Co-funding model, where public funding is dependent on the level of direct turnover based on contractual applied research.

5. Promotion of facilitator structures to speed up the launch of networking activities in order to better cope with their required transdisciplinarity and cultural diversity.

The success of promotion will not only necessitate solving scientific and technological issues but also taking into account the diversity of the objectives of university researchers, technology transfer partners and industry engineers in order to merge them into a common action which will benefit all. This merging action is indeed a bottleneck issue which requires highly skilled experts who are both recognised in academic as well as industrial activities. Among the various strategies to overcome this issue, the concept of facilitator structures is extremely interesting. It involves creating small public or private structures with a strong scientific expertise and a commitment for developing multidisciplinary research collaborations with non-academic partners. A few facilitator structures with synchrotron and neutron expertise play a discrete but very important interface role between large-scale facilities and companies. GENNESYS should try to promote these interface structures.

GENNESYS technology centres located at large-scale facilities throughout Europe

It becomes obvious that successful development of nanomaterial technology in Europe could profit from the set-up of clusters of excellence: "GENNESYS European Technology Centres". These centres could be organised as virtual and decentralised European institutes or as jointly operating on site laboratories. These European nano-/microtechnical laboratories could be the instrumental prerequisites to establish technologies of in-situ fabrication and characterisation of nano- and micromaterials, -structures, -components and -systems towards highly competitive European centres. The "GENNESYS European Technology Centres" could assure the efficient combination of advanced microscopy methods, fabrication- and processing tools and synchrotron radiation and neutron technology. These centres could be developed towards leading competence pools and towards cutting-edge user facilities of the European Union- and associated countries. They could give both internal and external users access to the key technologies at one-site strengthening the cooperation with universities, knowledge transfer centres and industrial research laboratories. A model for the GENNESYS European Industrial Platform for nanomaterials R&D&T is shown in Fig. 7.6.2. Networks are made between the various partners in the game: GENNESYS Technology Centres located at the large-scale facilities, industries, large- and medium-sized measuring facilities, European nanomaterials institutes and university laboratories.

The "GENNESYS European Technology Centres" could provide a broad arsenal of research tools for nanoscience and technology including a wide range of experimental equipment:
- Enabling the creation of extreme environments in which to explore the behaviour of nanomaterials and the synthesis of nanomaterials with extraordinary properties;
- Ranging from bench top-scale atomic force microscopes, used by

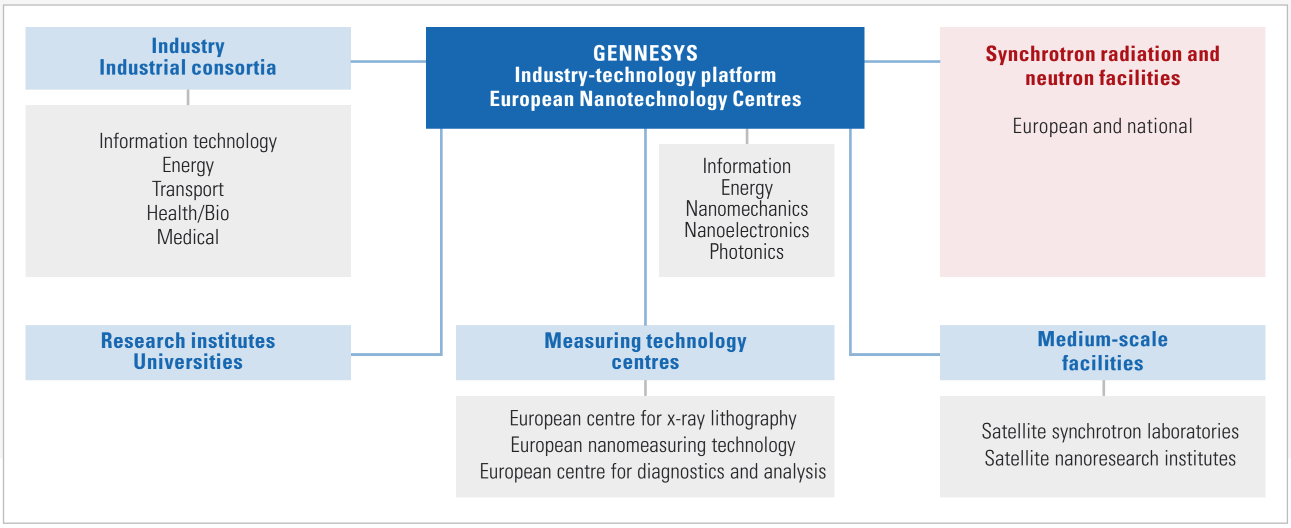


Fig. 7.6.2: GENNESYS industry-technology platform.

individual investigators, to large-scale test facilities generating synchrotron radiation and neutrons used by collaborative research and industry groups;
- Enabling new insights into systems of recognised importance and the exploration of completely new regimes.

The research field has advanced to a point that the large-scale facilities throughout Europe could become the ideal locations for partnership: for GENNESYS European Technology Centres which could be organised as jointly operated on-site laboratories and where it would be practical and possible to assemble in one place all of the intellectual resources and specialised equipment for a given research target.

These GENNESYS European Technology Centres would:
- Enable cross-disciplinary research;
- Leverage resources;
- Provide awareness of technologically drivers and potential applications;
- Enable extraordinary scientific and technological success through their ability to integrate long-term fundamental research, cross-disciplinary teams involving experimentalists, theorists, and nanomaterial synthesis and processing, and a strategic intent

The European Community should follow a well-balanced threefold strategy:

a) Support the establishment of new GENNESYS European Nanotechnology Centres optimised as supporting nanotechnology infrastructure and settled as satellite labs at suitable European and national large-scale facilities (Satellite-Nanotechnology-Lab at Large-scale facility);

b) Support the establishment of new GENNESYS European Medium-scale Facilities – that are decentralised medium size synchrotron facilities which are optimised as state-of-the-art working horse facilities – to be settled into European high-tech regions as satellite synchrotron labs near large nanotechnology institutes (Satellite-Facility at Nanotechnology Institutes);

c) Support the GENNESYS European Measuring Technology Centres for the development of small size synchrotron facilities for table-top measuring technology to be available in the nanotechnology labs and to be used for process-integrated non-destructive testing at the industrial production lines (Table-Top Facility at Industry).

The GENNESYS European Technology Centres could foster – or even be the prerequisite for – breakthroughs in a number of nanoengineering sciences, e.g.:
- GENNESYS European Nanocatalysts technology centre for the tailoring of new nanocatalyst materials: this is related to the discovery of new nanocatalyst materials and the invention of better processing techniques;
- GENNESYS European Nanocoating technology centre for the development of new coatings for aero-engine materials: this involves the optimisation of the nanocoating, and better coating deposition techniques and the understanding of degradation mechanisms in service (see the diagramme in Fig. 7.6.3);
- GENNESYS European Nanoscience technology centre for energy: discovery of nanomaterials to reach breakthroughs in new energy technologies as well as in conversion- and storage systems;
- GENNESYS European Nanoelectronics/photonics technology centre: a European medium-scale facility for x-ray lithography, diagnostics and analytical in micro- and nanoelectronics and photonics;
- GENNESYS European Technology Centre for Nanomeasuring Technology: for the development of table-top measuring techniques and instrumentation addressing in-situ inspection, nanodiagnostics and nanoanalytics of nanomaterials;

- GENNESYS European Centre for Nanomechanics for the study of the mechanical behaviour of materials on the nanoscale, with topics ranging from basic mechanical properties, residual stress, fatigue, cracks, supported by modelling to alloy design.
- GENNESYS European Nanohealth and Nanomedicine Centre to assess the inocuity of nanoparticles contained in the environment and consumer products and to open new routes in drug delivery and biomaterials
- GENNESYS European Soft-matter Nanotech Centre dealing with the design of high performance nanocomposite polymers and colloids and looking for enhanced quality and effectiveness of food and healthcare products.

GENNESYS – Industry technical platform

The creation of a GENNESYS-Industry technical platform in Europe around large-scale facilities, acting as an interface structure between "GENNESYS European Centres of Technology", the large test facilities throughout Europe, and the European companies, would become a necessity to:

- Bridge the gap between these two worlds: large-scale facilities and nanomaterial industry;
- Assure collaboration and coordination between the network of "GENNESYS European Technology Centres;
- Develop future industrial strategy for large-scale facilities and pinpoint centres of excellence;
- Develop European strategy for beam lines: research, process control, measuring developments, routine testing;
- Develop industry-dedicated beam lines;
- Manage the whole spectrum of industrial experimentation;
- Develop a European "nanomaterial" meeting point for industry and large-scale facilities.

The way from science to production requires managing and connecting different levels including:

- Curiosity-driven nanoscience;
- Exploratory technological research;
- Applied and industrial research and development;
- Industrial process integration, serial production of materials and devices including quality assurance

The organisation of GENNESYS – Industry partnerships

In order to encourage and foster scientific breakthroughs as well as business growth in the nanotechnology sector, the GENNESYS – Industry partnership should create a suitable climate for entrepreneurship and business development by providing the necessary means for joint research and development activities. This can be achieved by creating a GENNESYS Industry Council which will oversee the technology centres and interaction between the public and private sector as well as the large-scale facilities. The GENNESYS Industry Council will be composed of industrial members, the directors of the GENNESYS Science and Technology Centres, delegates from the European Commission, national organisations and industrial funding agencies, as well venture capitalists, and will direct the GENNESYS Industry organisation. The day-to-day management will be in the hands of a "general executive management" and a general director in charge of technical, communications, financial and commercial aspects. This is shown in Fig. 7.6.4.

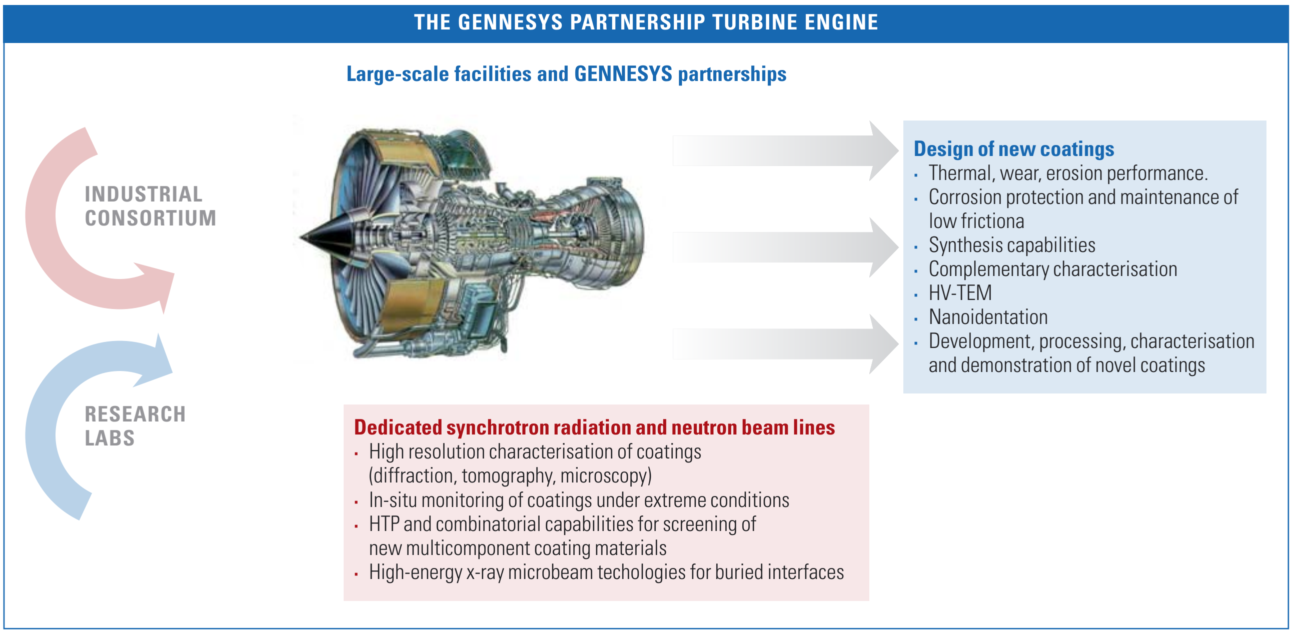


Fig. 7.6.3: Schematic of typical GENNESYS technology centre – in this case for nanocoating.

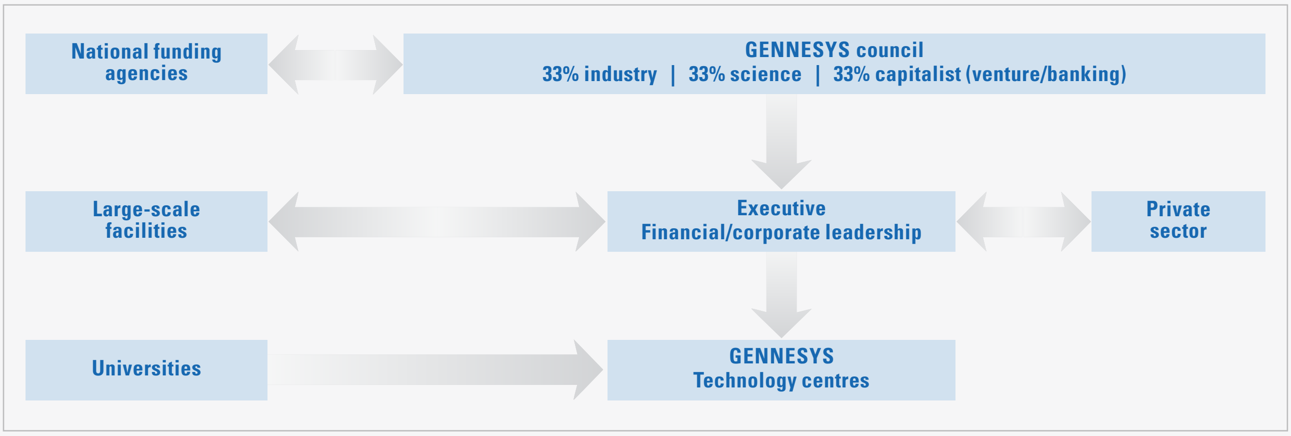


Fig. 7.6.4: The organisation of a GENNESYS industry council.

7.7. CONCLUSIONS

This exercise has identified a number of key issues as regards GENNESYS, from which the following conclusions in the framework of a wider European initiative based on the Lisbon agreement can be drawn:

- Cross-disciplinarity is the key to nanoscience and requires a multi-skilled workforce;
- Industrial research and development will benefit from stronger involvement in public research activities to capitalise on wide-spread intellectual property.
- The strength of large-scale facilities is unique in the techniques they offer and complement lab-based equipment.
- There should be a substantial increase in applied science oriented research programs at large-scale facilities, which may require significant changes in their operation and access modes.
- To this end, in order not to disrupt successful fundamental science programmes, publicly funded facilities should be strengthened and/or extended.
- Industrially relevant science programmes through partnerships with universities will ensure better training of the next generation of scientists, ensure lasting partnerships, provide technology transfer, and open up additional revenue streams through spin-offs, science parks etc.
- Academic and industrial research have been shown to work best through dedicated interface laboratories at selected sites (akin to science parks), and their development should be a high priority.

The success of GENNESYS-Industry will not only necessitate solving scientific and technological issues but also taking into account the diversity of the objectives of university researchers, technology transfer partners and industry engineers in order to merge them into a common action which will bring new benefit to all of them. This merging action is indeed a bottleneck issue which requires highly skilled experts who are both recognised in academic as well as industry activities. It will require:

- Involving as much as possible the industrial partners in the choices and decisions of GENNESYS-Industry, not only at the Council level but also in the task forces which will assess the needs and propose recommendations.
- Creating for each GENNESYS Technology centre an "Industry Advisory Committee". This committee will guide and advise for the development of the activities of the centre and will take care that they match the wishes of the industrialists.
- Relying on "facilitator" structures; a facilitator consists in small public or private structures with a strong scientific expertise and a commitment for developing multi-disciplinary research collaborations with non-academic partners. A few facilitator structures with synchrotron and neutron expertise already exists. They play a discrete but very important interface role between large-scale facilities and industrial companies. GENNESYS should try to benefit from their experience and involve them into its activities. A dedicated programme for launching new ones should also be prepared.

ANNEX I: TABLE-TOP SYNCHROTRON LIGHT SOURCES

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Over the past four decades, synchrotron radiation has made a revolutionary impact on many fields of science and technology. New windows to the micro- and nanoscale have been opened by using intense photon beams of x-rays, with many desirable properties, such as:
- Energy tunability;
- High peak and average brightness;
- Polarisation;
- Short pulse capability.

In addition to the contributions to basic science, the active and intense R&D effort at these large-scale facilities has resulted in new measurement techniques and technologies (e.g. x-ray optics) that are used in laboratories around the world. Furthermore, there has been a widespread economic and social impact from the introduction of new materials, new drugs and new applied disciplines originating in the synchrotron radiation community. Specifically on the application to nanotechnology, synchrotron radiation sources are critical for:
- Surface and interface characterisation;
- Nanopatterning;
- In-situ growth monitoring;
- In-vivo device testing (laser degradation mechanisms);
- Nanoscale x-ray probe for spatial resolution;
- Coherence effects.

However, the expense and size of large-scale facility light sources prevent synchrotron radiation technology from wide-scale availability to the private sector, smaller laboratories and university users. Numerous promising applications of synchrotron radiation cannot be accomplished on a practical scale, without a technological breakthrough towards lower cost, room-size devices, which would preserve the tunability, high spectral brightness and spatial resolution of the output x-ray beams. On the road towards commercially viable, compact synchrotron radiation sources, we consider three types of technological developments which can be accomplished over the course of the next decade:
1. Compact synchrotrons;
2. Inverse compton scattering light sources;
3. All-laser sources.

Radiation type	Wavelength or energy	Integrated photon power[1]
Far infrared (via synchrotron radiation)	10 – 50 µm	50 mW
EUV and soft x-ray (transition radiation)	80 eV – 1 keV	1 W
Hard x-rays (Bremsstrahlung)	10 keV – 20 MeV	100 W
Monochromatic (parametric) x-rays	8 – 20 keV	N/A[2]

Table 7-I.1: Compact synchrotron light sources.

1) Integrated radiation power over the defined range. Approximate maximum numbers given.
2) The performance of such machines for monochromatic x-rays has not yet been demonstrated.

Compact synchrotrons
Recently, a new class of compact synchrotron light sources has emerged that further reduces the size and cost (Tab.7-I.1).
They may be optimised for a variety of applications, including:
- Radiography for very high energies used in conventional NDT;
- Micro-tomography, microscopy and coherent imaging;
- Diffraction and scattering;
- Spectroscopy, including infrared;
- EUV-applications;
- Deep x-ray lithography;
- In-situ, in-laboratory studies of nanostructures.

Inverse Compton scattering light sources
Research in compact synchrotron x-ray sources has led to several design proposals for a compact x-ray source based on inverse Compton scattering (ICS) of an intense laser pulse from a relativistic electron beam. The efficiency of the ICS process increases greatly with laser field intensity, therefore very short pulses are often used (~ ps), which also has the effect of producing x-rays of very high peak brightness. Further increases in flux will come over time from progressive technological improvements in accelerator and laser repetition rate as by the use of superconducting linacs, which are capable of achieving very high repetition rates (> 1 MHz), matching the performance of solid state lasers. Recent designs are targeting 10^{12} ph/s at 12 keV for protein crystallography.

Laser accelerator light sources
For several years, high peak power lasers have been used to interact with a plasma to produce x-rays. These sources produce x-rays when a high-intensity laser is focused onto a solid or gas. The plasma contains electrons up to 1 keV, and nonlinear mechanisms produce even higher energy particles. The resulting x-ray spectrum from the source contains both bremsstrahlung and K shell radiation, with time-scales approximately equal to the laser pulse duration. These sources, however, have comparatively low peak and average brightness, are not tunable (spectrum peak depends on the material), and are limited in photon energy (< 8 keV). Ongoing development efforts are working on increasing the brightness of such systems.

The most promising route towards table-top synchrotron radiation sources is an all-laser ICS or FEL system, which use a small footprint, ultra-high gradient laser accelerator to produce a beam of high energy electrons, which subsequently interacts either with a laser or a magnetic undulator. Given the rate of advancement of laser systems, such a device could become very inexpensive and compact in the future.

Roadmap: 2008 – 2020: for table-top synchrotron radiation machines (Fig. 7-I.1)
It is perceived that the true technological breakthrough will occur as the high peak brightness, high repetition rate ICS technology will merge with the all-laser systems. An important step in this evolution will be improvements in the repetition rate, reliabilility and tunability of laser

accelerators. One of the premier application of table-top synchrotron radiation systems will be x-ray microscopy (see Table 7-I.2). In the meantime, other technologies will play important roles in bringing industry, research labs and synchrotron radiation community together in an effort to introduce small-footprint, low cost synchrotron radiation devices.

Conclusion

In conclusion, while truly table-top laser-based synchrotron radiation sources are still immature, they present an opportunity for significant scaling of both the cost and size of future light sources. Although synchrotron radiation has become an extremely powerful tool in science and technology today, it has not yet had the impact on society the invention of the x-ray tube had more than 100 years ago. In order to reach this level, compact synchrotron radiation sources must be developed so that the costs can be reduced to a level where medium-sized companies or large hospitals could afford the acquisition of such a facility. Furthermore, the reliability must be at least 95% and the maintenance costs should amount to no more than one or two technicians. A 'killer' application could be either medical imaging or medical therapy, if such new sources combined with x-ray microscopy could deliver significantly improved diagnoses or treatment compared to what is currently possible. The facility must be run by a hospital and its staff and the price per treatment must be of the same order of magnitude as competing techniques. In order to reach such a goal, a compact light source must first be developed, which is most likely to happen within the next 2–3 years. Secondly, its reliability and long-term performance must be tested simultaneously with the development of new x-ray techniques specifically developed for the source. Thirdly, if a medical application is to be targeted, further clinical tests must be done – these can be time-consuming. Hence, for technical applications, compact synchrotron sources could hit the market 3–5 years, whereas a widespread medical application would take 5–10 years.

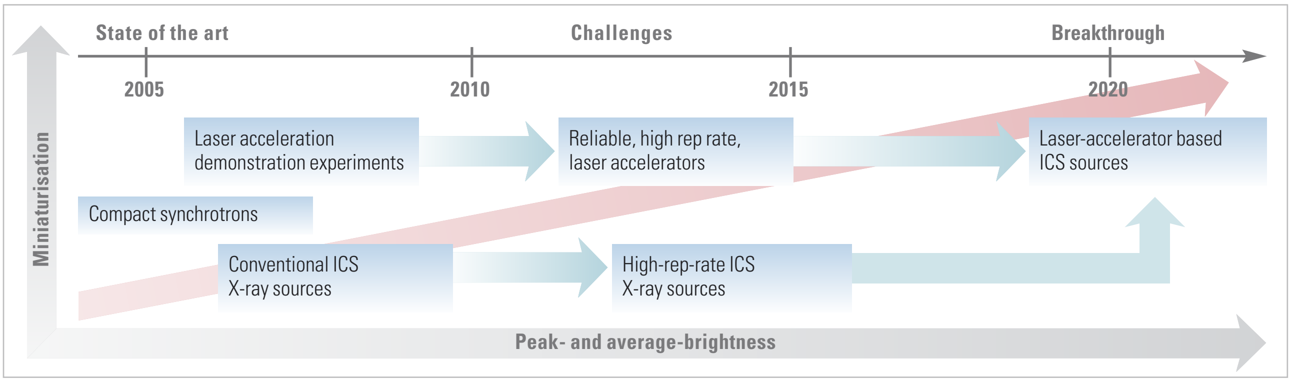

Fig. 7-I.1: Roadmap for table-top synchrotron radiation machines.

	LIGHT MICROSCOPY	TEM	TXM
Imaging beam energy	A few eV	10 keV to 1 MeV	Multiple keV
Resolution	100-200 nm	A few nm	25 nm
Penetration depth	Many mm	< 1 μm	Hundreds of μm
Sample preparation	Simple, in-situ and in-vivo observation	Difficult; section and metal coating usually required.	Similar to light-microscope, in-situ observation possible
Radiation damage to sample during imaging	Almost none	High; limited number high-resolution images even with cryo-stabilisation	Low; can acquire many images with resolution < 50 nm at room temperature
Imaging environment	Room condition	Vacuum required	Room condition for 2-D imaging. Cryogenic condition for 3-D tomographic imaging
3-D imaging (resolution: transverse × longitudinal)	Optical sectioning of whole cell. Assemble numerically (200 nm × 500 nm)	2-D transmission imaging of physically sectioned cells. Assemble images numerically (5 nm × 100 nm)	Tomographic imaging of whole cell or tissue samples. Reconstruct numerically. (30 nm × 30 nm)
Co-localisation with light microscopy	–	Difficult	Easy 3-D co-localisation with built-in visible-light microscope
Function-specific imaging	Large selection of labels with fluorescence microscopy. Multiple labelling	Gold particle labels	Dark-field or phase-contrast microscopy, multiple labelling possible. Quantum dots for fluorescence microscopy

Table 7-I.2: Comparison of imaging properties of visible-light, electron microscopes, and the transmission x-ray microscope.

ANNEX II: INDUSTRIAL APPLICATIONS OF LARGE-SCALE SYNCHROTRON RADIATION AND NEUTRON INSTRUMENTS FOR ADVANCED MICROELECTRONICS

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The down-scaling of minimum dimensions of silicon-based CMOS technologies enables the integration of an increasing number of transistors on a single chip, as described by Moore's law. For more than four decades, Moore's law has driven the rapid pace of improvement of the CMOS transistor-based products and the research and development activities of the microelectronics industry. This trend has changed recently and is represented graphically in Fig. 7-II.1.

The vertical axis refers to the scaling:

- Geometrical scaling: the continued shrinking of horizontal and vertical physical feature sizes of the on-chip logic and memory storage functions in order to improve density (cost), performance (speed, power) and reliability values;
- Equivalent scaling: 3-D device structure, non-geometrical techniques and new materials that affect the performance of the chip, and novel design techniques and technology (multi-core design);
- When the CMOS reaches its ultimate limits, even with the integration of new materials to replace the silicon channel, i.e. around 2020, the "beyond CMOS" approach will intent and develop a new information processing technology to eventually replace CMOS.

The horizontal axis refers to "More than Moore's" law and relates to functional diversification. It consists of the incorporation into microelectronic devices of functionalities that do not necessarily scale according to "Moore's law" but provide additional value to the end-user: The "More than Moore" approach typically allows for the non-digital functionalities: RF communication, power control, passive components, sensors, actuators.

Even if the weight of the "More than Moore" component of the microelectronic industry evolution increases over time, the main industrial applications of synchrotron radiation and neutron facilities for the microelectronics industry will concern the down-scaling of CMOS transistors ("Moore's law") down to the 22 nm and 16 nm generations in 2016 and 2019 respectively.

It will require the:

- Introduction of new materials as:
  - Gate dielectrics (high permittivity dielectrics: high κ);
  - Gate electrodes (metals, metal silicides or nitrides) for multi-gate CMOS;
- High carrier mobility materials (Ge, III-V…)
- Engineering of stresses at the gate level for improving the mobility of carriers in the CMOS channel, and, consequently enhancing transistor performance;
- Control of the hydrogen distribution, which can passivate dangling bonds, reduce stresses, impacting device performances;
- Introduction of lower and lower dielectric constant dielectrics (low κ) for insulating Cu metal lines, since the device performance will be highly susceptible to increases in propagation delay, cross-talk noise and power dissipation of the Cu interconnection structure;
- Use of thinner and thinner diffusion barrier layer for enhancing the electrical conductivity of Cu lines in narrower lines;
- Control of thermomechanical stresses in Cu interconnects for ensuring excellent reliability of the microelectronic devices.

Consequently, the combined introduction of new materials and the continuous thinning of the transistor constitutive layers will generate huge challenges for analytical characterisation techniques. These characterisation techniques (Fig. 7-II.2) should be able to provide the following:

- Local analytical characterisation of chemical, structural, electrical and atomic bonding at the nanometre/atomic scale;
- 2-D and 3-D information, since 3-D effects will become more and more important with transistor down-scaling;

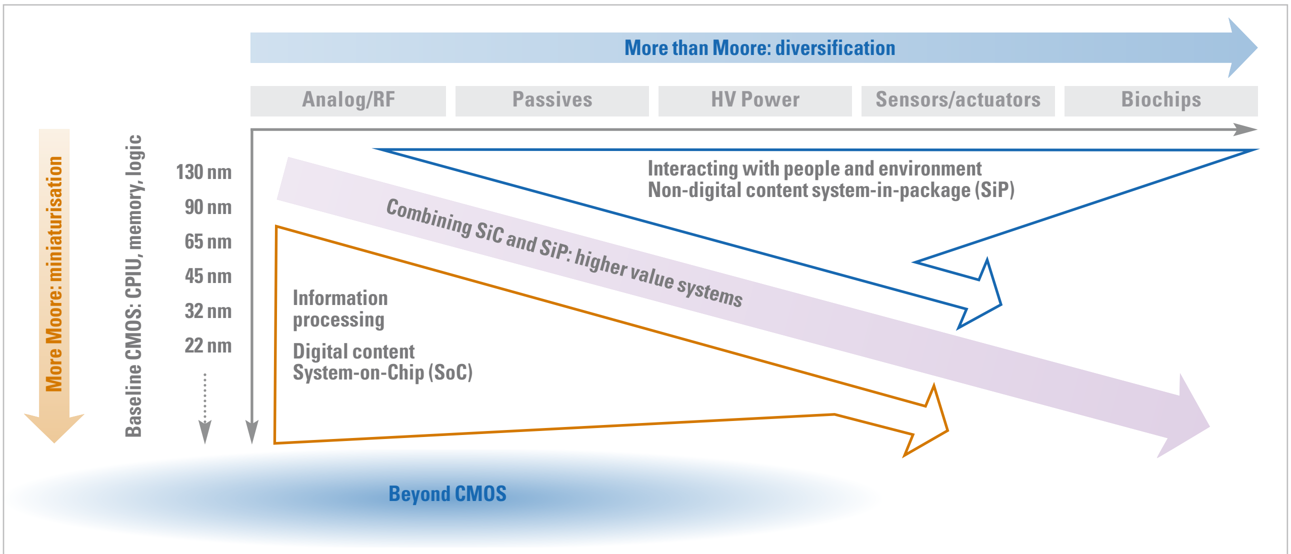

Fig. 7-II.1: Moore's law and more.

- Spatial (lateral, depth) resolution close to the 0.1 nm range: atomic resolution;
- Atomic sensibility for detecting any fluctuation of a physical or chemical property;
- Sub-surface and interface characterisation.

In order to support research and development activities devoted to the development of advanced CMOS transistors, techniques available at large-scale synchrotron radiation and neutron facilities can be favourably used for characterising (Figs. 7-II.3 and 7-II.4):

- Chemical properties of the buried interfaces between the silicon or non-silicon channel, the high κ film and the gate electrode: HR-XPS and EXAFS;
- Distribution of hydrogen in high κ/metal electrode film stack: Neutron reflectivity combined with x-ray reflectivity;
- Distribution in NMOS and PMOS channels: nanospot XRD;
- Defects induced by the ion implant process steps: GI-SAXS.

When it will be available, x-ray scatterometry (CD-SAXS) will be very useful as a calibration technique for the in-line CD metrology equipments.

The R&D activities and a periodic monitoring of technologies related to Cu/low κ interconnects can be supported by the following techniques based on synchrotron radiation:

- Cu film texture and Cu grain size: μ-spot XRD;
- Strain distribution in Cu lines: μ-spot XRD;
- Chemical characterisation of the interaction at the porous low κ/thin barrier: Cu interfaces: HR-XPS, EXAFS;
- Pore microstructure of low κ dielectrics: GI-SAXS.

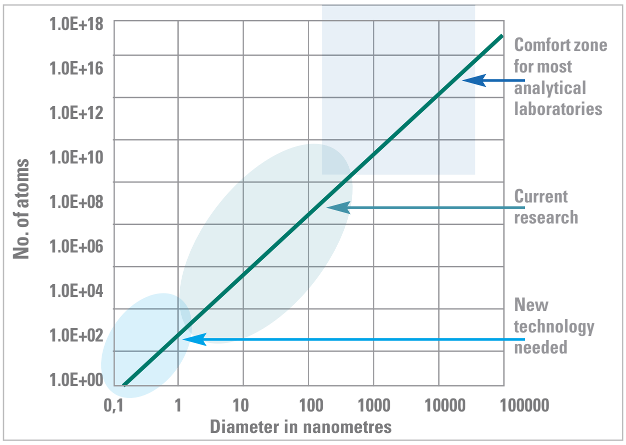

Fig. 7-II.2: Compulsory evolution of the analytical characterisation.
Courtesy: E.M. Vogel, 2005 Proc. characterisation and metrology for ULSI technology.

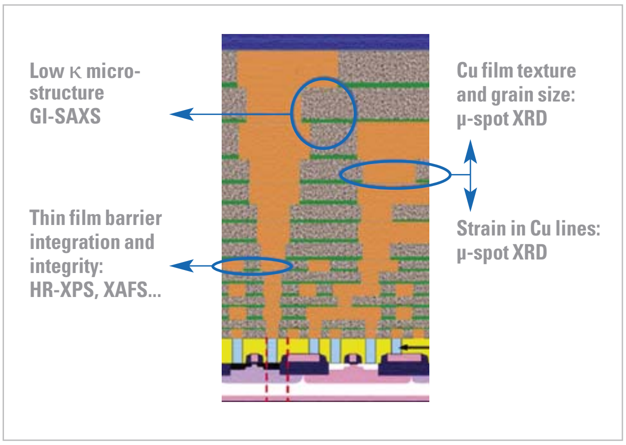

Fig. 7-II.3: CMOS transistor-BEOL.

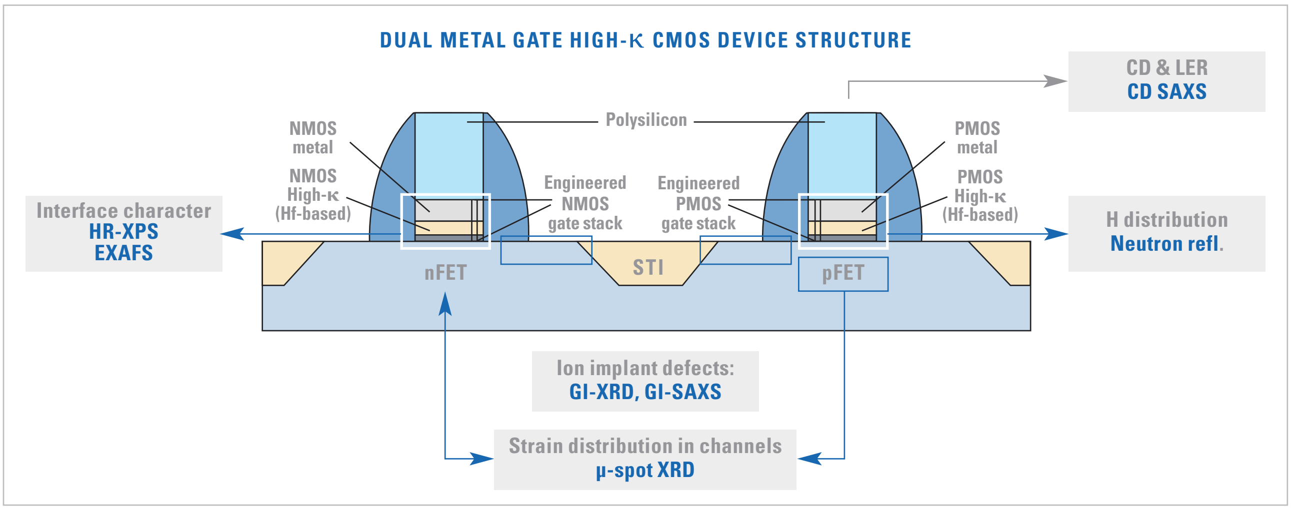

Fig. 7-II.4: CMOS transistor-FEOL.

8. FUTURE IMPLICATIONS OF GENNESYS FOR EUROPEAN SYNCHROTRON RADIATION, LASERS AND NEUTRON FACILITIES

8.1. OVERVIEW

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The development of synchrotron radiation and neutron sources for the fine analysis of matter has been pioneered in Europe. During the last 2 decades, an enormous analytical potential has been built up which must be better exploited to meet the grand challenges in nanomaterials development. Today, Europe has an impressive network of synchrotron radiation and neutron facilities.

Neutron facilities*	Location	Thermal power	Number of beam lines
BENSC	Germany	10	32
BNC	Hungary	10	10
FRM-II	Germany	20	27
ILL	EU (France)	58	34
ISIS spallation source	UK	-	26
JEEP-II	Norway	18-25	??
LLB	France	14	23
RID	Netherlands	2	3–4
SINQ spallation source	Switzerland	-	19
FRG-1 closing 2009	Germany	5	

*(alphabetic order)

Synchrotron radiation and x-ray laser facilities*	Location	Electron energy (GeV)	Number of beam lines
ALBA (1st phase)	Spain	3	7
ANKA	Germany	2,5	15
BESSY	Germany	1,8	21
DIAMOND	UK	3	27
DORIS III	Germany	4,5	20
ELLETRA	Italy	2,2	26
ESRF	EU (France)	6	32
European XFEL Hard x-ray laser 1st Phase in construction, start 2013	EU (Germany)	20	3–5
FELBE IR Laser	Germany	0,04	2
FLASH Soft x-ray laser	Germany	0,45	3
ASTRID II	Denmark	1,4	
MAX IV in construction, start 2009	Sweden	1,5/3	14
PETRA-III in construction, start 2010	Germany	10	14
SLS	Switzerland	2,4	17
SOLEIL	France	2,75	
SRS closing 2008	UK	2	11

*(alphabetic order)

Fig. 8.1.1: List of European synchrotron radiation and neutron facilities.

In the preceding chapters of this document, materials scientists have put together the future breakthroughs in nanotechnology as well as the emerging key barriers which have to be overcome by the analysis of nanomaterials and nanomaterials phenomena on the atomic level. In order to meet these future challenges in the fine analysis of nanomaterials, the already available advanced techniques – STM/AFM, TEM, x-ray and neutron technologies, and NMR – must be tailored to the particular needs of materials scientists. In addition, novel analytical tools have to be conceived (such as XFEL), and complementary techniques have to become merged together to allow for new insights into the nanoworld (see Fig. 8.1.1).

Today, advanced x-ray and neutron techniques, as provided by the modern European facilities, are applied to current problems in physics, chemistry, medicine and in biological science as well as in environmental and engineering sciences. These techniques are extremely important for the non-destructive in-situ analysis of nanomaterials.

The entire portfolio of analytical technology may be subdivided into:

- (X-ray and neutron) diffraction (elastic scattering) to extract surface, subsurface and bulk information on the nanostructure, chemical composition, magnetic ordering, as well as stresses and strains of the nanomaterial under investigation;
- Absorption spectroscopy to investigate the short-range environment around selected atomic species;
- Photoelectron spectroscopy to interrogate the electronic structure of nanomaterials;
- Inelastic (neutron and x-ray) scattering which probes the excitations of the sample (lattice vibrations, electronic and magnetic excitations);
- Quasielastic neutron scattering and neutron spin-echo experiments to sample slow dynamics such as diffusion and magnetic fluctuations;
- (X-ray and neutron) reflectometry to interrogate the structural and magnetic density profiles within processes in thin films, coatings, buried interfaces and multilayers;
- (X-ray and neutron) imaging and microscopy to obtain information from nanostructures directly in real space;
- (X-ray and neutron) tomography to obtain 3-D images of the element distribution within nanomaterials and nanodevices.

In order to exploit this enormous analytical technology for overcoming key barriers in the development of new nanomaterials, the following must be developed:

- Dedicated instrumentation with an adequate sample environment (pressure cells, furnaces, cryostats, reaction cells, shear cells, etc.);
- Highly accurate sample positioning devices;
- Efficient detectors with fast count rates and high spatial precision;
- The necessary infrastructure for data acquisition, data storage and data analysis.

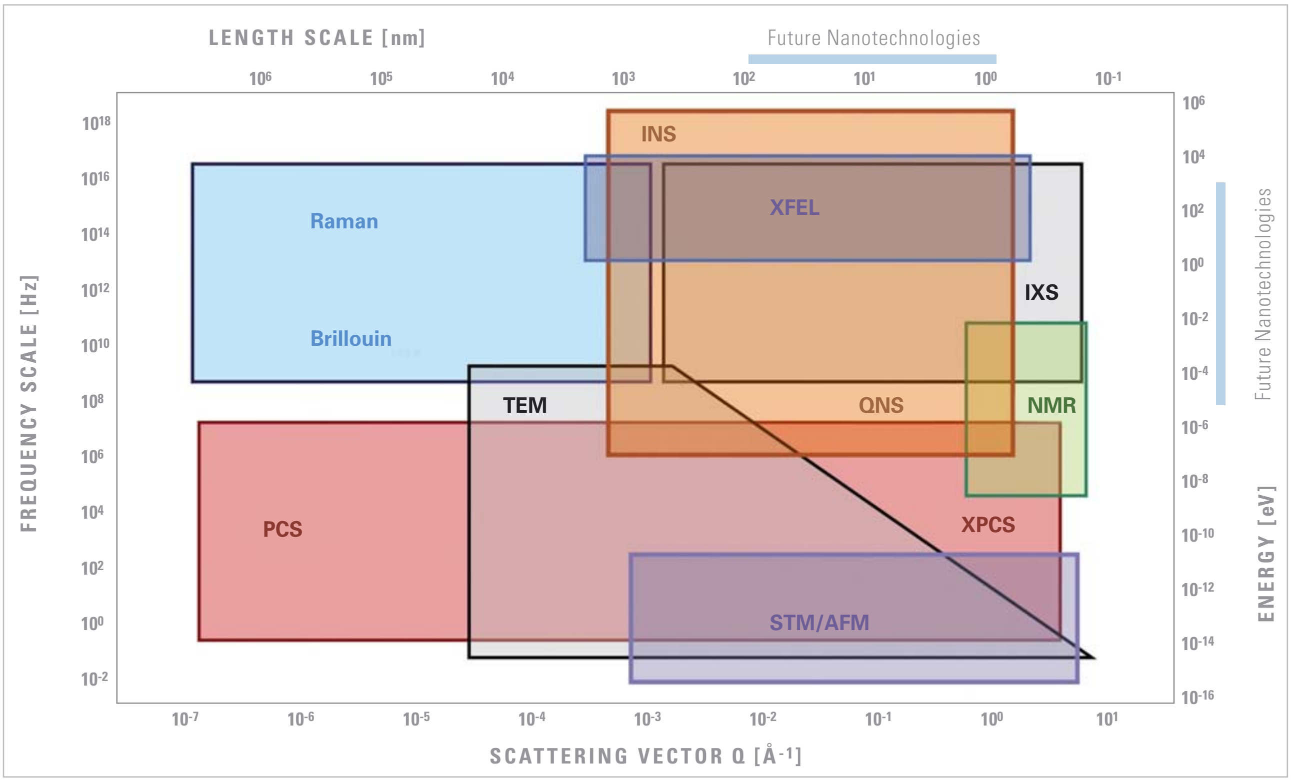

Fig. 8.1.2: Advanced analytical techniques for nanomaterials (AFM = atomic force microscopy, INS = inelastic neutron scattering, IXS = inelastic x-ray scattering, NMR = magnetic resonance, QNS = quasielastic neutron scattering, STM = scanning tunnelling microscopy, TEM = transmission electron microscopy).

8.2. NEUTRON FACILITIES

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Currently, more than 8 dedicated neutron facilities with well-established user programmes are operational in Europe. Here, the energies of neutron beams exploitable for nanomaterial research range from a few nano-eVs up to eVs. The corresponding neutron wavelengths cover the full range from sub-atomic to super-molecular spacing. This means that scattering experiments can provide information over a wide range of length scales – from some 10^{-1} nm to 10^{4} nm. Analysing any change in energy of the neutron as it interacts with matter can inform us about both the slow motion of polymers and the fast excitations in electronic systems. In particular cold neutrons, with energies in the range of 0.5 to 5 meV, are an unparalleled tool to investigate fluctuations on timescales from a few ps up to nearly µs.

Interactions of neutrons with matter are weak, simple, non-destructive and easy to analyse; they are such that neutrons penetrate deeply into matter. This allows for a straightforward use of even complex and bulky sample environments and leads to extremely good statistical averaging over the sample, as required by several of the task forces for characterisation procedures in material research and industry. Nevertheless, this does not prevent neutrons from being highly sensitive. It is, for example, possible to investigate minority components of a sample down to a few ppm. Neutrons are equally very well-suited to the study of films and interfaces of atomic thickness. The fact that information obtained through neutron scattering is undistorted makes it ideally suited for a comparison with theoretical calculations. This closing of the knowledge cycle is pre-eminent in many of the task force recommendations.

Neutrons "see" nuclei of atoms, rather than the diffuse electronic charge distributions. This leads to major advantages, such as being able to detect light atoms in the presence of heavy ones and to vary contrast between chemical elements via isotopic substitution. In particular, task forces dealing with hydrogenated materials such as polymers or biomaterials have identified the need for further development in this area.

The neutron has an intrinsic magnetic moment ideally suited to probe even tiny magnetic moments (0.01 μ_B/atom) carried by electrons or by nuclei. Most of what is known about magnetic structures comes from neutron diffraction. Neutron polarisation methods offer exquisite magnetic sensitivity and enhanced tools for energy analysis.

Building on the inherent strength of the technique, neutron facilities all around the world profit from new technology in upgrading the performance of their resources and instruments. The upgrade of these facilities is encouraged by the efforts of the user community to propose smarter experiments on cutting-edge science. In the past decade, this process has attained an impressive speed. Improved flux and higher resolution (both in space and time) allow for increasingly precise measurements on increasingly smaller (0.001 mm^3) or more dilute (10 ppm) samples, or allow faster kinetic studies. Clever manipulation of the neutron spin leads to new ways of exploring surfaces and interfaces. Dedicated infrastructure makes neutrons accessible to engineers and biologists. Fig. 8.2.1 gives a description of the advances achieved in neutron scattering during the past decade and those to be expected in the near future. A completely new dimension of experiments can be predicted for the second-generation spallation sources that are presently under construction in both the USA and Japan.

As already mentioned, the interplay of facilities and users is essential for progress in neutron scattering. There are already working examples of such collaborations in several scientific areas including engineering and biology. However, regarding materials research in the broad sense as defined by GENNESYS, the full integration of laboratories and facilities has still to be accomplished. Dedicated sample environments, and maybe even complete spectrometers, as well as on-site expertise are required to exploit the full potential of this powerful technique. The task forces have all clearly pointed in this direction. In addition, in-situ integration with other experimental probes, such as differential scanning calorimetry, x-rays or optical spectroscopy, is clearly called for.

QUANTITIES MEASURED-ANSWERS, LIMITS OF DEDICATION & RESOLUTION	
SPATIAL DIMENSIONS	**TIME SCALES**
Smallest sample volume .001 mm^3 Shortest measurable atomic displacement 10^{-3} nm Largest particle 0.1 mm Chemical sensitivity 10ppm Magnetic sensitivity 0.01μ_B/Atom Magnetic moment direction 0.5 deg	Shortest spectroscopy 10^{-15} s Longest relaxation time 10^{-6} s Best kinetics time resolution 10^{-3} s Temporal stability: years

Fig. 8.2.1: Current and anticipated achievements in real space and realtime (neutrons).

The technical requests for analytic tools made by the task forces can be translated into a set of precise instrumental requirements for the facilities. These include, for example, the need for fast time-resolved investigations, or the already mentioned combination of the neutron experiment with other experimental probes. These requirements will be addressed below and compared with present or future possibilities.

Apart from technical questions, beam access is a crucial question brought up by all the task forces. A guaranteed number of beam 'days' no longer meet the users' requirements. New schemes have to be developed which incorporate the notions of confidentiality, continuity, and on-time access.

8.2.1. NEUTRON METHODS AND FUTURE CHALLENGES

In the following section, we will briefly present the neutron methods relevant for GENNESYS and discuss their specific impact in revealing important information to the materials scientist.

Neutron diffraction

Diffraction studies allow locating the mean positions and the associated magnetic moments of atoms in a sample. The technique is applicable to single crystals, textured materials, polycrystalline powders and disordered matter.

Time-resolved and stroboscopic diffraction

Because of their high penetrating power, neutrons have long been important for following real-time chemical and electrochemical reactions in large volumes. For example, the chemical processes inside a real battery can be followed, as the battery is charged/discharged; the hydration/dehydration of minerals, or the absorption/desorption of gases in zeolite catalysts, can be studied in the bulk. As neutron diffractometres become faster thanks to focussing optics, bigger detectors and new sources, it is becoming possible to measure on shorter timescales, typical of many chemical reactions. Recent examples include 'self-propagating high temperature synthesis' of new ceramic materials, where the self-propagating reaction can be followed on a 300 ms timescale (see Fig. 8.2.2).

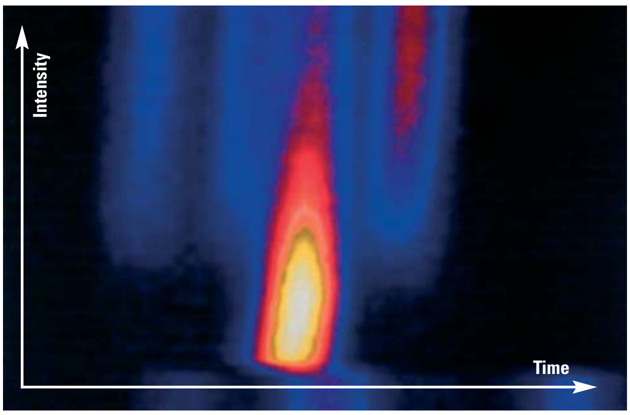

Fig. 8.2.2: Self-propagating reaction monitored by time-resolved neutron diffraction.

Stroboscopic (repetitive) experiments applied to reversible reactions and transitions will allow time resolution and data acquisition within 30 microseconds (the travel time for neutrons through the sample ultimately limits the time resolution to around 10 microseconds).

Texture and spatially resolved diffraction

"Texture" denotes the preferred orientation of the nanocrystals that often determine the strength of materials ranging from minerals to metal or ceramic engineering components and living teeth and bones. The penetrating power of the neutron means that this nanocrystalline texture can be mapped out in 3-D for large objects, simply by measuring the relative numbers of neutrons reflected from different atomic planes.

Measurement of stress and strain

Internal stresses are decisive for the strength and lifetime of almost any work piece. Neutrons penetrate deeply into structural materials such as steel, aluminium or titanium (several cm for steel or several 10 cm for aluminium) and are thereby ideally suited for the non-destructive measurement of internal stresses. Internal strains can be mapped out by measuring small changes in the inter-atomic spacing. New highly intense beams will permit the study of volumes between 0.1 mm^3 (typical case) and 0.001 mm^3 (best case). Typical samples will range from welding to soldering joints to work pieces like cylinder heads and the combustion chambers of Ariane space rockets. X-ray methods are complementary in that they can be used on smaller components or near the surface with a higher level of resolution. Future materials include metal alloy materials, but also composite materials, carbon or silicate fibres, ceramics and polymers. Most materials will be nanostructured, however in cases like turbine blades, the opposite holds – they will be almost single crystalline. Future instruments will accommodate large work pieces >1m^3 , allow in-situ applications of cyclic or steady state external loads and temperatures up to the 3000°C region. Engineers will be the typical users of these instruments, and services including fine data analysis will become routine.

Small Angle Neutron Scattering

Small Angle Neutron Scattering (SANS) is a well-established technique to examine structures on length scales of 1 to 100 nm. Given the unique penetration depth of neutrons, SANS is a powerful method to investigate aggregation phenomena and the morphology of functional materials and systems including: amorphous solids; porous materials; magnetic or nanostructured alloys; colloidal particles; functional polymers; biomembranes; protein complexes; or molecular machines. Magnetic phases and static and dynamic behaviour of magnetic nanomaterials can be probed with polarised neutron SANS. Composition, structure and aggregation of ferrofluids in-situ or magnetically alignable membranes can be resolved and characterised.

Contrast variation by isotopic exchange allows for the specific enhancement and visualisation of substructures in complex nanocomposites. Phase transitions, self-assembly and aggregation mechanisms in the synthesis and formation of nanomaterials can be followed in real-time experiments down to 1 s time resolution and below at current high flux SANS instruments. Measurements at extreme conditions of pressure, temperature and magnetic field are easily accessible to SANS investigations.

Surface scattering

Since their introduction 20 years ago, neutron surface scattering techniques have been improved continuously. Neutron specular reflection can be used to probe thin film multilayer structures down to a length scale of a few nanometres and has now become a routine technique. More recently, off-specular reflectivity has been made available to mainstream users for the probing of in-plane structures in the micrometre range (1–50µm). At present, Grazing Incidence Small Angle Neutron Scattering techniques are being developed in order to probe planar nanostructures in the 5 nm–200 nm range. This panel of techniques thus allows us to probe thin film structures over a huge length scale (5nm–50µm), in all reciprocal space directions.

The large neutron penetration depth allows the resolution and study of buried structures and hidden interfaces down to sub-µm depth. In-situ aggregation and self-assembly of nanoparticles near interfaces in solution or melts can be probed, which allows molecular-level processing at interfaces for functional nanostructures and nanotechnology.

Neutron fluxes are still limited, especially compared with x-rays, and so these techniques should only be used in cases where neutrons bring a distinct advantage. These fields are: (a) polymer and biological systems studies where isotopic labelling can provide unique information; (b) solid/liquid and liquid/liquid interfaces for which the low neutron absorption allows simple set-ups; (c) magnetism of thin films for which neutron reflectivity has been an invaluable tool in the last decade.

Neutron surface spectrometres now offer a wealth of sample environments e.g. temperatures in the range of 1 K – 1000 K; stability down to 0.01 K; 6 T magnetic fields; Langmuir-Blodget cells. The main problems materials scientists currently face are linked to:
(a) The requirement for high quality samples, especially flat samples, which are not always compatible with materials science processes;
(b) The long measuring times (typically several hours per sample) which prevent systematic parametric scanning with respect to external parameters (temperature, pH, magnetic field).

Techniques to resolve these problems mostly rely on improved use of the neutron beams. Existing reflectometers only use a tiny fraction of the neutron phase space (wavelength – divergence). New techniques based on the parameterisation of the neutron beam with an extra variable (the spin) allow better use of the neutron phase space to be made. These gains can be used either to probe "non-perfect" samples, or to enhance the available resolution down to Q ~$6 \cdot 10^{-3}$ nm^{-1} without losing flux. Further progress is also expected in the field of polarised neutron reflectivity, which is benefiting from new technologies such as polarised ^{3}He spin filters. These advances will be essential in future spallation sources. Time-resolved experiments are technically possible but are facing a flux issue. Nevertheless, in stroboscopic mode, millisecond time resolution could possibly be achieved. In "single shot" experiments, the most optimistic timescales are in the one-minute range, which may prove useful in some cases. These considerations lead us to say that the future of neutron surface scattering techniques looks bright and that significant breakthroughs will certainly be achieved in the near future.

Neutron spectroscopy

Neutron inelastic scattering is a unique tool to explore the time domain between microscopic atomic vibrations and macroscopic processes in condensed matter. This time domain corresponds to 10^{-12} – 10^{-6} s, which can be covered by a suite of neutron scattering instruments, primarily time-of-flight (TOF), backscattering and Neutron Spin Echo (NSE) spectrometers. There is a natural correlation between the time and length scales of processes in matter. On the one hand, larger and therefore heavier objects naturally move more slowly than lighter ones, so nanometre-sized objects, such as biological macromolecules or segments of polymer molecules tend to move around in a flexible environment on the ns timescale, while the motion of atomic size objects is characterised by fs timescales. On the other hand, it takes longer for atomic size objects to move over longer distances, and again nanometre distances will often correspond to ns times, well in the middle of the range covered by quasielastic scattering techniques.

Atomic and molecular motion on the nanometre scale can play a crucial role both in the formation of nanoscale structures and in their functionality. For example the formation of micellar structures by self-organisation in solutions is related to the elastic properties of the micellar segments, or the viscoelastic properties of polymer melts is controlled by the motion of polymer chains constrained by neighbouring molecules. Quasielastic neutron scattering can follow nanoscale processes not only in time, but also in space, over distances from a fraction of a nanometre to about a few nanometre. For example, the diffusion of atoms or molecules can be conveniently determined over such short distances by this technique. In nanostructured materials this might be all the room available for the atoms to move around and the diffusive motion needs indeed to be observed locally, in very restricted volumes. Similarly, neutron spectroscopy can monitor the dynamics of magnetic nanoparticles (anisotropy, relaxation times) in the femtosecond to microsecond timescales.

Neutron imaging

Historically, radiography by neutrons was one of the first applications of neutron beams. Today it is among the strongest growing application of neutrons in materials science. The reasons for this are manifold: once again, neutrons easily penetrate several 10 cm into almost all kinds of materials. Tremendous progress has been achieved in detecting neutrons fast and on large two-dimensional areas. Today, large, two-dimensional detectors detect neutrons in 100 time slots with a spatial resolution of 50 x 50 m^2. Dedicated instruments at the world's most intense continuous neutron sources are under construction to provide spatial resolutions down to the μm scale. They are equipped with wavelength selectors in order to sharpen contrast at the Bragg edges of different materials. Pinholes as small as 0.5 mm allow for phase contrast imaging. Latest instrumentation uses neutrons for the high level of contrast they provide, namely thermal (meV) and fast (MeV) neutrons, thereby allowing the privileged imaging of hydrogen containing work pieces. This progress is currently being implemented in neutron tomography, i.e. the 3-dimensional imaging, of technical parts. Owing to the ideal contrast of neutrons, technical objects can be decomposed into all their different materials in a completely non-destructive manner.

Time-resolved radiography will detect the combustion in a running engine in time slots of 100, contrast variation will make the distribution of H_2 and H_2O visible in running fuel cells on the m scale, fine archaeological objects will be decomposed into their different contents without being touched (see Fig. 8.2.3). For engineers, geologists, archaeologists, neutrons will become the light in the dark, making visible objects which have until now remained invisible.

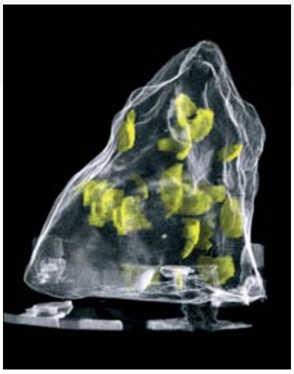
Fig. 8.2.3: Monkey tree leaves embedded in a 56 million year old fossil.

Neutron characterisation of nanomaterials

Neutron methods have established themselves as a key tool for the analysis of materials. Depending on the problem to be addressed, the different length scales, timescales or geometries in real space, various neutron methods/techniques are exploited. In the following, we present the links between GENNESYS Task Force groups and neutron methods.

8.2.2. FUTURE CHALLENGES FOR NEUTRON FACILITIES

The existing neutron facilities are upgrading their neutron infrastructure but also their interfaces with users. ILL and ISIS have launched major upgrade programmes of their neutron sources and instruments; PSI in Switzerland and LLB near Paris are renewing their neutron equipment. The new reactor near Munich, FRM-2, has recently started its user operation.

Moreover, the neutron centres are developing the infrastructure needed to host engineers and scientists that are not trained in neutron methods. Properly interfacing neutron and synchrotron centres with their industrial communities will optimise the use of beam time: engineers can prepare their measurements with the help of neutron experts (procedures, strategy, metrology). Furthermore, neutron users will receive full on-site support for the data acquisition and data analysis. Such peripheral facilities will include micromanipulation and characterisation of samples as well as proper software and instrument control methods in such a way that the operation of dedicated neutron instruments for nanosciences is made routine and high-throughput.

Nanomaterials scientists are welcome to make use of large-scale facilities to obtain fast and reliable answers to their engineering problems. Industrial access to the neutron centres requires that the neutron facilities make quick access to neutron beam time guaranteed on relevant instruments to the whole community. In this respect, neutron facilities in Europe should consider pooling their neutron resources in order to optimise investment and operation of neutron beam lines and facilities.

AREAS IN NANOMATERIALS SCIENCE AND TECHNOLOGY		DIFFRACTION	LOQ	INELASTIC SCATTERING	IMAGING
FUNDAMENTAL SCIENCE	Synthesis	•	•		
	Nanostructures		•		
	Functions	•	•	•	
	Modelling				○
NANOMATERIALS DESIGN	Structural materials	•	•		
	Functional materials	•	•		•
	Bio-nanomaterials		•		•
	Engineering		•	•	•
	Reliability		•		
NANOMATERIALS TECHNOLOGY	Nanoelectronics				
	Health	•			•
	Nanomechanics	•			•
	Transport				
	Chemical industry	•		•	
	Energy	•		•	
	Petrochemistry	•		•	•
	Environment	•			
LINKS WITH INDUSTRY	Access	•	•	•	•
	Confidentiality	•	•	•	•
	Standards	•	•		

Table 8.2.1: Relevance of neutrons to nanomaterials science and technology I.

	ANALYTICAL NEEDS	NEUTRON TECHNOLOGY
SURFACES AND INTERFACES	Depth dependence	Specular reflectometry,
	Lateral structures	Off-specular reflectometry
	Magnetism	Polarised neutron reflectometry
	Catalysts	Diffraction, time-resolved diffraction, in-situ experiments
SYNTHESIS	Intermediates	Time-resolved powder diffraction, stroboscopic data acquisition
	Polymer synthesis	SANS
BIOASPECTS	Precise location of H atoms	Diffraction, deuteration
	Morphology	SANS, reflectometry, selective isotope labelling
	Motion-function relation	Inelastic incoherent/coherent scattering
	Membranes	SANS, reflectometry, D-labelling
THIN FILMS	Film growth, diffusion	Reflectometry, GISANS
	Wetting, aggregation coatings	
HIGH SURFACE AREA MATERIALS	Adsorption	Diffraction, time-resolved
	Catalysis	Spectroscopic studies of reagents and intermediates
	Diffusion	Quasi-elastic scattering
FUNCTIONAL MATERIALS	Material processing	Time-resolved diffraction, stroboscopic studies
	Imaging	Time-resolved radiography
	Characterisation (size, shape distributions)	SANS
	Diffusion (conducting polymers)	Quasi-elastic scattering
STRUCTURAL MATERIALS, CONSOLIDATED MATERIALS Steel, concrete, alloys, composite materials	Characterisation	Diffraction, stress-strain and texture analysis, tomography
	Time evolution	Time-resolved diffraction, tomography
INFORMATION TECHNOLOGY	Nanostructured array, buried layers	Polarised Neutron Reflectometry, GISANS
	Magnetic roughness	High resolution TOF
	Molecular clusters, spin dynamics	Diffraction
	Magnetic phase diagrams	Reflectometry, GISANS
NANOBIOTECHNOLOGY, HEALTH	μ-fluidics	SANS, reflectometry
	Drug and gene delivery	High resolution diffraction, deuteration
	Active sites	Per-deuteration and neutron crystallography
	Protein-protein interactions	Neutron tomography
AERONAUTICS AND MECHANICAL ENGINEERING	Process monitoring	Strain-stress analysis
	Failure analysis: strain in industrial size objects	Texture analysis
	Anisotropy of mechnical properties	SANS and reflectometry
	Coatings	Diffraction, spectroscopy
ENERGY AND ENVIRONMENT	Catalysis	High resolution spectroscopy
	Ionic conduction	Diffraction
	Hydrogen storage	Diffraction, neutron spectroscopy
	Clathrates	Powder diffraction
CHEMISTRY	Active sites	Time-resolved diffraction
	Reactions	Deuteration and diffraction, spectroscopy
	Hydrogen bonds	Numerical modelling
PRE-NORMATIVE RESEARCH	Standards	Absolute microscopic measurements on all accessible scales
		Reproducibility

Table 8.2.2: Relevance of neutrons to nanomaterials science and technology II.

8.3. SYNCHROTRON RADIATION AND LASER FACILITIES

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[Affiliations chapter 12]

Synchrotron radiation is produced by ultrarelavistic electrons in the GeV regime which are forced by tailored magnetic field arrays to radiate highly collimated x-ray light. Within the last two decades, synchrotron radiation technology has developed into an indispensable tool of condensed matter science. Synchrotron radiation has a broad field of applications, in physics, chemistry, materials-, life-, earth-, and environmental science, touching upon many aspects of everyday life. There is a large variety of experimental techniques exploiting synchrotron radiation that is well-established for the investigation of nanophenomena and nanomaterials and characterise and monitor nanodevices.

8.3.1. STATE OF THE ART

Currently, Europe boasts more than 10 dedicated operational synchrotron radiation facilities specialised in the spectral range of hard x-rays and having a well-established user programme. Current synchrotron radiation techniques encompass diffraction, diffuse scattering, spectroscopy, microscopy, tomography, topography and combinations thereof which are based on several unique properties of synchrotron radiation that complement those of other probes, such as electron microscopy, tunnelling microscopy and neutron spectroscopy. The most prominent properties of x-rays and in particular synchrotron radiation are the following:

- Low scattering cross section allowing easy data interpretation and the application of rigorous theories for quantitative conclusions (exception: dynamical diffraction from perfect crystals) unique potential for non-destructive testing and for in-situ analysis of materials.
- Continuous wavelength spectrum covering the electronic spectrum of matter allowing photoelectron and absorption spectroscopy to yield the electronic and chemical properties of a specimen while x-ray fluorescence yields its chemical composition with unparalleled sensitivity.
- Bulk and surface sensitivity allowing both access to surface properties, buried nanostructures and bulk properties;
- Unique potential for non-destructive testing and for in-situ analysis of materials;
- Circular and linear polarisation for the radiation allowing the investigation of magnetic properties and phenomena;
- Large penetration depth of hard x-rays into matter, allowing the investigation of the internal structure of materials and of materials inside specialised sample environments (high pressure cell, a furnace or cryostat), strong magnetic fields, or inside a chemical reactor.

Recent developments in x-ray optics have made it possible to produce nanometre sized x-ray beams for structural, chemical, and elemental information either spatially resolved on the nanoscale from inside a specimen or within a specialised sample environment for in-situ studies. Current and future synchrotron radiation technologies are therefore ideally suited to address the urgent scientific questions in nanomaterials research pointed out in chapters 2 to 6. However, in order to develop their full potential, they require the most brilliant x-ray sources and the most efficient optics and detectors.

8.3.2. FUTURE NEEDS

X-ray nanobeam technologies at synchrotron radiation facilities are still at an early stage. To make x-ray nanobeams routinely available to users in nanomaterials research, they need to be developed further in particular in the hard x-ray range, requiring major improvements of the following:

- X-ray source;
- X-ray optics;
- X-ray detectors;
- Experimental (sample) environment;
- Ancillary equipment for (nano-) sample handling and preparation;
- Access to synchrotron radiation sources and training of users.

European research infrastructure in the future

To implement x-ray microscopy and time-resolved spectroscopy techniques, brilliant x-ray sources are required providing pulses with the shortest possible duration. Synchrotron radiation sources are currently the most brilliant hard x-ray sources available, having evolved quickly over the past few decades (see Fig. 8.3.1).

As the demand for nanoscale investigations and time-resolved studies increases, these sources are in need of further upgrade to

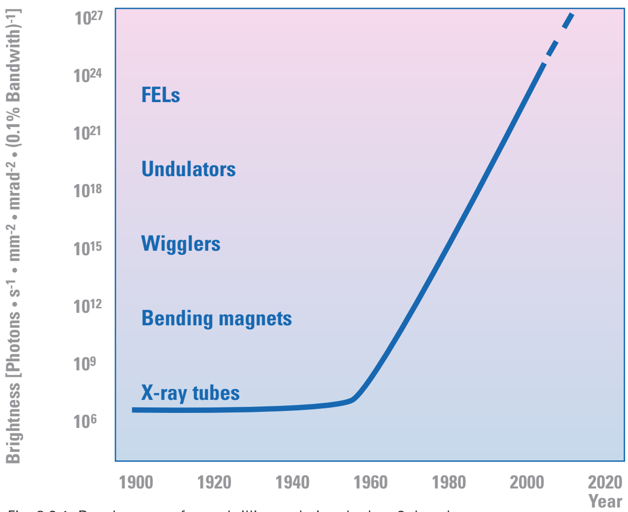

Fig. 8.3.1: Development of x-ray brilliance during the last 2 decades.

optimise them in view of these applications. In addition, the development of novel x-ray sources such as free-electron lasers or energy recovery linacs has to be pursued. The following synchrotron radiation source developments are currently in a tangible planning phase:

- Optimal use and upgrade of existing storage rings, including ESRF (EU), BESSY (GER), Elettra (I), SLS (CH).
- Optimal use of the FLASH free-electron laser facility for the spectral range of the EUV and soft x-rays (GER)
- Design of new 3rd generation storage rings with nanobeam capability, including DIAMOND (UK), PETRA III (GER), SOLEIL (F), ALBA (ESP), MAX-IV (S).
- Design of the European X-ray Free-Electron Laser XFEL (EU) The XFEL will provide a dramatic increase in brilliance and extremely short x-ray pulses in the range of a few 10 fs. This radiation is ideally suited for nanobeam technologies (incl.x-ray microscopy) and time-resolved studies.
- Conceptional studies of the Energy Recovery Linear accelerator (ERL) which will provide – along with the appropriate x-ray optics/ x-rays beams of ultimate properties – for nanomaterials development. Currently, design studies for the ERL concept are being carried out at Cornell University (USA) and at Argonne National Laboratory (USA). There is no comparable European project.

X-ray optics for nanoscience and nanotechnology

Currently, there is a variety of x-ray optics available for microscopy and nanoimaging based on diffraction (e.g. Fresnel zone plates and multilayer mirrors), refraction (e.g. refractive x-ray lenses), and reflection (e.g. mirrors based on total external reflection). The smallest foci reached today lie between 20 and 50 nm (see Fig. 8.3.2). Currently, the performance of all x-ray optics is technology limited, and ultimate physical limits of the spatial resolution seem to lie well below 10 nm.

For future use in nanomaterial development, it is mandatory that necessary mechanical stability and accuracy of the critical beamline components are developed and implemented. Currently, there are several hard x-ray nanoprobes that can stably provide a spatial resolution of about 100 nm. Stable focusing of hard x-rays to below 20 nm should be feasible in the mid-term. In the long run, focussing to 5 nm and below is targeted.

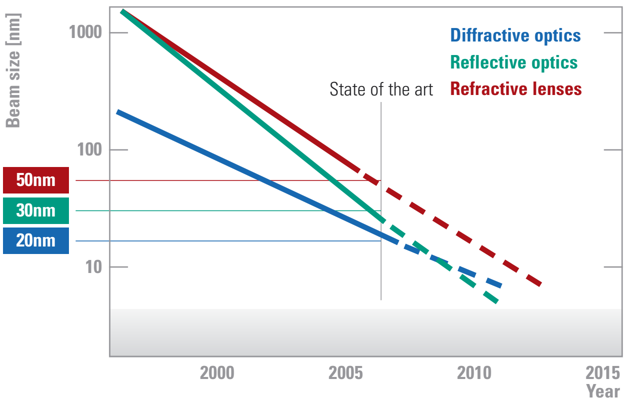

Fig. 8.3.2: Development of the x-ray beam size for different x-ray optics.

Optics	Bent/curved mirror	Bent/curved multilayer	Waveguide	Fresnel zone plate	Refractive optics
First realisation	Kirkpatrick, Baez (1948)	Underwood, Barbee (1986)	Feng et al. (1993)	Baez (1952)	Snigirev et al. (1996)
Energy	> 30 keV	> 80 keV	< 20 keV	< 20 keV	< 5 keV - 1 MeV
$\Delta E/E$	white beam	10^{-2}	10^{-3}	10^{-2} – 10^{-3}	10^{-2} – 10^{-3}
Dispersion	none	$\sim\lambda$		$\sim\lambda$	$\sim\lambda^{-2}$
Focus achieved	30 nm	41 nm	25 nm	19 nm	47 nm
Theoretical focussing limit	$\approx$15nm	$\approx$5nm	< 10 nm	< 1 nm	< 5 nm (2nm)

Fig. 8.3.3: Comparison of different x-ray optics and achievable x-ray beam cross-sections.

X-ray detectors

For many x-ray applications, the detector is still the limiting factor. For an efficient future implementation of x-ray nanobeam technologies (as microscopy) and in particular ultrafast studies, improved detectors are mandatory. Currently, there are several developments of fast, massively parallel detectors with a high level of efficiency and dynamic range. These prototypical detectors are only an answer to some of the experimental demands. Furthermore, they are available at only a few beam lines and will have to be made available to the community to efficiently contribute to the GENNESYS project in the future. Even with the newest detectors, there remain many unfulfilled experimental requirements, imposing the need for further developments. Since the development of detectors is expensive and requires long-term commitment, a concerted effort at the European level is essential for this development to make effective use of it at the various sources in Europe. This is even more important for experiments at next generation sources, such as the XFEL. At the same time, sufficient funding and mechanisms for efficient dissemination and commercialisation of the developed detectors must be made available.

Experimental environment

- **Sample environment**

In order to make optimal use of the beam time at synchrotron radiation sources, the necessary infrastructure to prepare and characterise samples is required. For nanomaterials science, micro- and nanomanipulation, as well as investigation and characterisation of the sample by other microscopy techniques are needed such as optical, scanning electron (SEM), and scanning probe microscopies (e.g., AFM and STM). Some of these tools are already being successfully used at current synchrotron radiation sources. They are becoming more and more important with the growing nanoprobe activities at these large-scale facilities. In addition, it will be increasingly important to provide the possibilities for preparing and handling nanomaterials at the large-scale facilities, whether in-situ or ex-situ.

- **Computing capabilities**

Computing resources and software for data storage and data processing have become paramount. While the computing resources have grown steadily with the demands for efficient data storage at third generation synchrotron radiation sources, users of the facilities are often required to evaluate the data themselves. In particular in x-ray imaging, large amounts of data are generated that need to be processed further. In order to make these techniques available to nanomaterials scientists that are not experts in the field of x-ray imaging, automatic data evaluation is required.

8.3.3. RECOMMENDATIONS AND CONCLUSIONS: NANOMATERIALS SCIENCE NEEDS FOR THE UP-GRADE OF LARGE-SCALE FACILITIES

The following measures are needed to make optimal use of synchrotron radiation facilities for nanoscale materials science in the future:

- In order to be internationally competitive in nanoscience, European synchrotron radiation sources need to be optimised for high brilliance and stability. Significant improvements over synchrotron radiation sources in terms of brilliance and time structure are expected from free electron lasers and energy recovery linacs (ERLs). Currently, there is no European project comparable to the US-ERL projects in Cornell and Argonne, USA, and the project pursued at KEK in Japan. Thus, there is the danger of a future technological gap in accelerator technology for x-ray science.
- The XFEL offers unique opportunities for nanomaterials science, especially for time-resolved studies in the femtosecond domain. The Euro-XFEL is in a good position in the international context. However, to make optimal use of this facility, a lot of instrumental and methodological developments are needed.
- Optics are currently limited by technology: technological developments are needed in particular in metrology and nanofabrication in order to improve their performance, both in terms of efficiency and imaging quality. In addition, fundamental research in x-ray optics is needed to probe the physical limits of x-ray microscopy.
- Detectors are currently a major limiting factor for nanoscience applications at synchrotron radiation sources: fast and massively parallel detectors optimised for detection quantum efficiency, spatial resolution, and dynamic range are needed, in particular in view of nanoscience applications at x-ray free-electron lasers.
- A concerted effort at the European level is required to dedicate and optimise synchrotron radiation beam lines for nanoscience applications. This includes optimisation of the beam lines for optimum performance, improvement of the stability of all beam line components, and high precision mechanics. In order to make optimal use of x-ray microscopy, special sample environments for in-situ studies compatible with nanoprobe techniques are needed, such as high pressure cells, miniature chemical reactors (microfluidics), cryostats, ovens, or magnets.
- Ancillary services must be made available in the vicinity of nanoprobe beam lines for sample preparation and characterisation. The possibility for automatic data evaluation and modelling of experiments needs to be provided in order to attract users who are not necessarily experts of the experimental technique, but need it as a tool for their science.
- Facilitate access to beam time for both research laboratories and industry. This may include new scheduling schemes to allow for on-time access. In addition, special training of users should be made available to facilitate the access to these sources.
- Improve awareness of the potential of synchrotron radiation techniques for nanomaterials science in industry and the public.
- Improve training of university scientists and future industrial users.

European Science Centre for x-ray nano-optics

Nanoscale materials research at synchrotron radiation facilities requires sophisticated instrumentation. Aside from a brilliant source and efficient x-ray detectors, x-ray optics are crucial to nanoscale science investigations at synchrotron radiation facilities. The growing demand for nanoscale science research at European synchrotron radiation sources creates an equally growing need for high quality x-ray optics and their reliable supply. Continuously evolving nanotechnological advances demand more and more sophisticated nanoanalytics, requiring continuous improvement of x-ray optics. Theoretical considerations suggest that the ultimate fundamental limits to focusing lie well below 10 nm. At present, x-ray optics are technologically limited, meaning that significant advances in optics development can still be made.

The fabrication of cutting-edge nano-optics requires extremely specialised know-how and high-end nanofabrication tools currently only available at large-scale research facilities and academic institutions. In order to go beyond the current state-ofthe-art in x-ray nano-optics development, a joint European effort is needed. In view of the significant cost of the relevant top-level technologies, it is essential to focus the efforts in leading institutions, minimising redundancy. The role of the 'European Science Centre for X-ray Nano-optics', therefore, is to coordinate the necessary joint efforts of future x-ray nano-optics regarding the following points (see Fig. 8.3.4):

- Design and simulation;
- Fabrication;
- Testing and metrology;
- Commercialisation.

The needs for x-ray optics are specified by nanomaterials research at synchrotron radiation sources, serving as input for the design and simulation of x-ray optics. The resulting fabrication routes developed at nano-optics fabrication facilities are validated by the testing of prototypes using metrology at radiation sources. The centre promotes the commercialisation realised either by the transfer of newly developed fabrication technologies to existing companies in the field or by founding start-ups from the institutions involved.

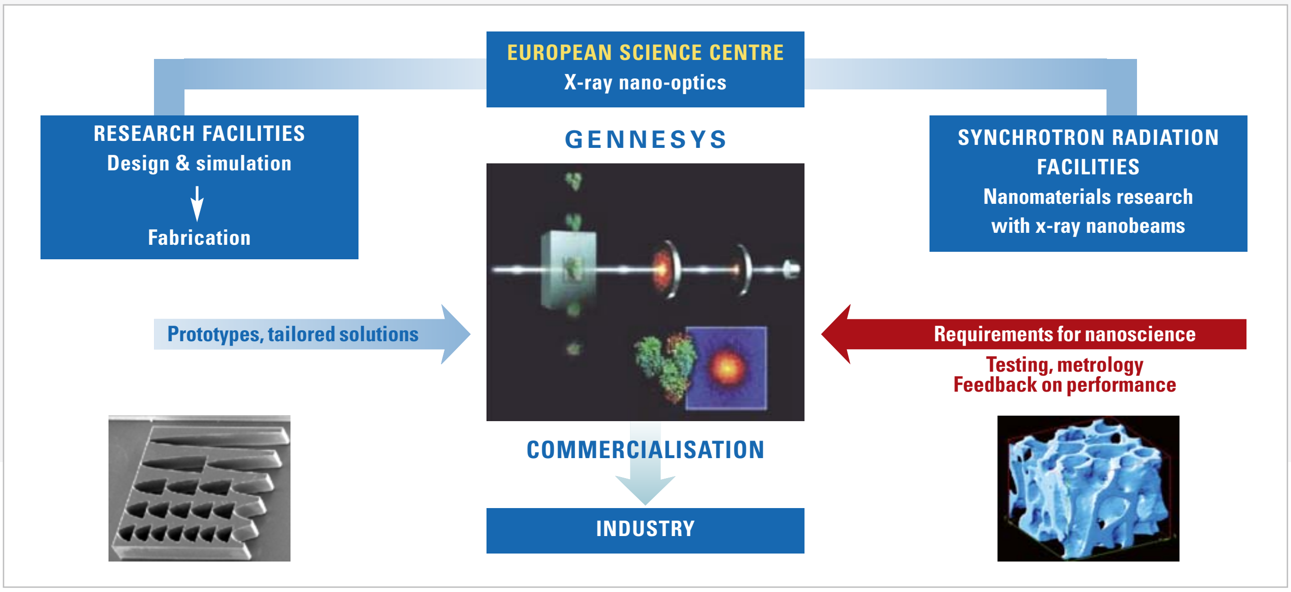

Fig. 8.3.4: Workflow inside the European science platform for x-ray nano-optics.

European Science Centre for Development of Advanced Detector Systems (x-rays and neutrons)

In the past, detector development has evolved at a slower pace than the developments in sources and optics. As already stated in different chapters of this document, the development of advanced detector systems is crucial in reaching the research and technology goals addressed in this initiative. Today's challenge is the development of large-area, high efficiency, high-counting-rate x-ray detectors (see Fig. 8.3.5). Furthermore, fast silicon-based detectors and gas detectors for spatially-resolved and time-resolved experiments are increasingly in demand. In this respect, very large investments in terms of capital costs and manpower are necessary, requiring budgets that are often well above any single institute's resources. As a consequence, Europe-wide or even worldwide collaborations are in the pipeline and these collaborations should receive as much reinforcement as possible. For this, large-scale facilities in Europe can play a coordinating role, since these rely quite heavily on the capabilities and knowledge of participating institutions. During the past few years, it has been remarked that a cross-disciplinary effort involving both experts from particle physics and astrophysics having a long track record in successful detector development, is most promising.

APPLICATION AREAS		
Imaging	Diffraction	Time-resolved experiments
Pixel detectors CCD cameras	Pixel systems Microstrip system	Gas-filled devices Avalanche photodiodes
TECHNOLOGY CHALLENGES		
Pushing the limits towards large area, high efficiency, high dynamic range, short read-out times, high spatial resolution		

Fig. 8.3.5: Detectors, application areas and technology challenges.

A non-exhaustive list of systems in different phases of development includes:

- Pixel detectors for imaging and diffraction;
- Microstrip detectors for diffraction;
- Pixelated avalanche photo diodes;
- Advanced CCD systems for imaging.

- **Pixel and microstrip detectors**

Hybrid pixel detectors, which have been used for modern high-energy experiments, are now under development to fulfill the requirements imposed by the high flux and brightness of the newest synchrotron radiation facilities. The most important features of hybrid pixel single photon counting detectors are: read-out speed, no dark current/read-out noise resulting in a high dynamic range, very good point spread function, quantum efficiency and large sensitive area. The systems currently under development (Medipix, PILATUS, Mythen) are composed of hybrid modules, that can be arranged either in a linear or rectangular array. Operating in single-photon counting mode with a threshold discriminator, noise-free recording of x-ray images is feasible. Main fields of application are powder diffraction, crystallography, surface diffraction and imaging with a resolution of the order of the pixel size (50 to 150 microns, depending on the system). But the field of application is not limited to x-ray detection. Sensors coated with ^{157}Gd were used to produce a module sensitive to thermal neutrons while modules without a sensor layer have been used for both electron and visible-light detection.

Further developments are urgently needed:

- Decrease in the pixel size (while still keeping a radiation tolerant design);
- Increase in the framing rate, aiming at read-out frequencies up to ten kHz;

- Development of GaAs sensors, in order to improve efficiency for higher photon energies;
- Development of 3-D chip integration.
  (This allows one to stack together multiple chips by using chip connection technologies. This technology is of extreme interest and value for building segmented x-ray detectors, for instance one can construct a stack of an analogue signal processing chip, a digital signal processing chip, a large memory chip, and an optical communication chip. It allows one to construct pixel detectors, with functionality limited only by physical limits that can be tiled together with minimal gaps.)

- **Avalanche photodiodes**

Based on an international collaboration, developments for the construction of an APD array for photon correlation experiments has been started. In the short term, the prototyping of a linear array is envisaged. Mid-term strategy is the realisation of a two-dimensional array. This system should aim at high detector efficiency, high counting-rate capability (dead times shorter than 4 ns), high dynamic range and high spatial resolution.

- **Gas detectors**

For the investigation of time-lapsed experiments in diffraction and applications in soft-condensed matter research, the development of space and time-resolved gas-filled detectors should be strengthened.

- **Advanced CCD systems**

In the last few years, significant advances in the field of CCD-based detectors have been made. These detectors cover a broad range of applications in imaging and have been adapted for special applications such as parallel data acquisition in spectroscopy. However, in order to improve the efficiency of CCD based detectors, it is important to develop and produce converter screens (scintillators) using higher-Z elements like the newly introduced GGG.

- **New detectors for XFEL nanoscience**

For the envisaged time-resolved coherent x-ray diffraction/imaging studies of nanomaterials on ultrashort time scales (sub-picoseconds), novel pixel detectors must be developed. A joint European detector development plan is mandatory in order to exploit the full potential of future x-ray lasers for nanomaterials investigations.

- **Diamond detectors for beam monitoring**

For efficient use of the experimental stations, it is increasingly important to monitor the incident beam, both in intensity and in position (direction). With the ever decreasing beam size (improved focussing) and with the wish to preserve the beam coherence, currently used beam monitors are no longer adequate.

The enormous challenges facing us in the development of novel detection systems for synchrotron x-rays, neutrons and XFEL x-rays which fulfill the stringent requirements in quantum efficiency, dynamic range, spatial and temporal resolution in order to leverage the potential of the large-scale facilities for nanomaterials science and technology can only be solved by a European joint effort (Science Centre for Detector Development) which integrates expertise from different fields and embarks on a sustainable cooperation with other worldwide activities in this field (see Fig. 8.3.6).

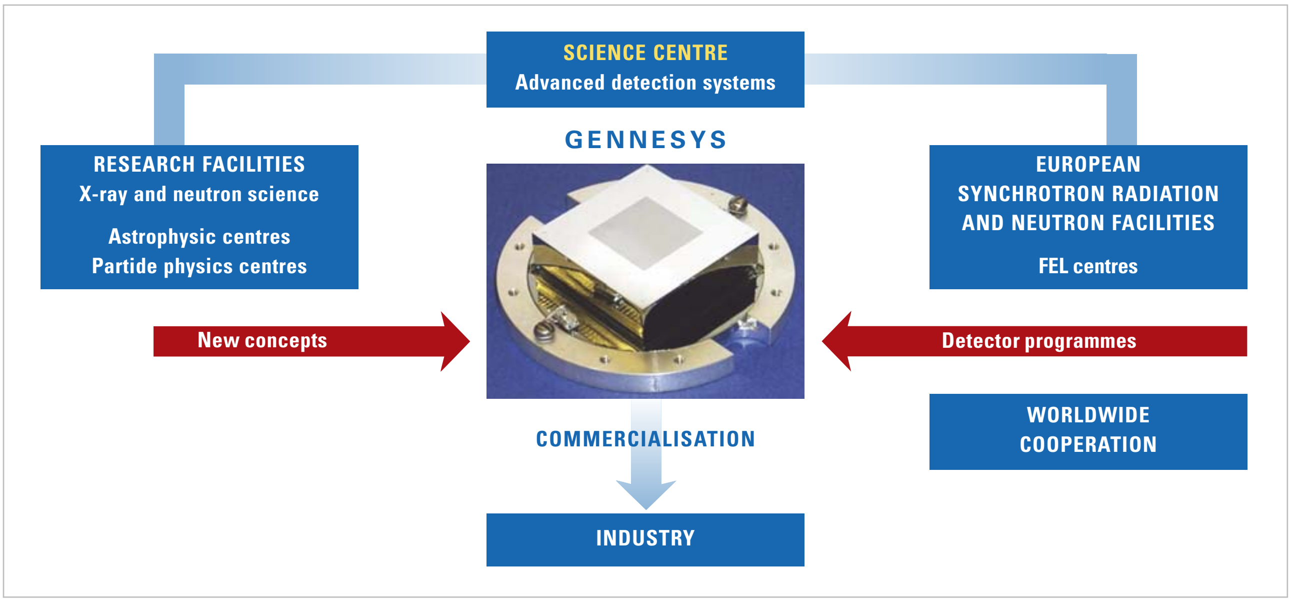

Fig. 8.3.6: Science centre for advanced detection systems.

8.4. CONCLUSIONS

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[Affiliations chapter 12]

Future role of European synchrotron radiation and neutron facilities for the development of nanomaterials and nanotechnology

European large scale facilities for analytical testing provide:

- Dedicated experimental stations with sophisticated analytical specifications;
- Different sample environment ranging from clean ultravacuum chambers, high pressure cells, cryostats, high temperature furnaces to growth chambers and electrolytic cells;
- Reliable, stable and strictly reproducible experimental conditions;
- Transparent user access based on scientific excellence;
- Local contacts for advice before the experiment and direct assistance during the experiment;
- Support for young and untrained scientists.

The GENNESYS initiative has brought to light that the future analytical barriers for the development of nanomaterials for new technologies can only be overcome if the demands of nanomaterials science and the analytical potential of synchrotron radiation and neutron sources are brought together for new breakthroughs in nanomaterials synthesis, functions and modelling.

Nanomaterials development at megafacilities: In order to leverage the various analytical technologies developed at the European large-scale facilities for the development of nanomaterials and nanotechnologies, GENNESYS has initiated crossover action between the different scientific disciplines and sectors all over Europe (see Fig. 8.4.1 and Fig. 8.4.2).

Based on the results and conclusions of this study, it is mandatory that several sustainable actions at synchrotron radiation and neutrons are initiated, i.e. the development of:

- Joint focused European projects for nanomaterials development;
- Provision of specialised Support Labs on site for nanomaterials design, nanomaterials handling, complex sample environments
- New experimental stations on the specific demand of nanomaterial science (converging and combinatorial techniques);
- New experimental stations on the specific demand of nanotechnology industry (standardised, remote-control, high throughput, safety);
- A dedicated training programme (see Chapter 9);
- Build-up of nanoscience and nanotechnology centres;
- Novel pulsed x-ray (free electron lasers) and neutron sources (spallation sources) for access to fast and ultrafast phenomena and processes in nanomaterials and -devices.

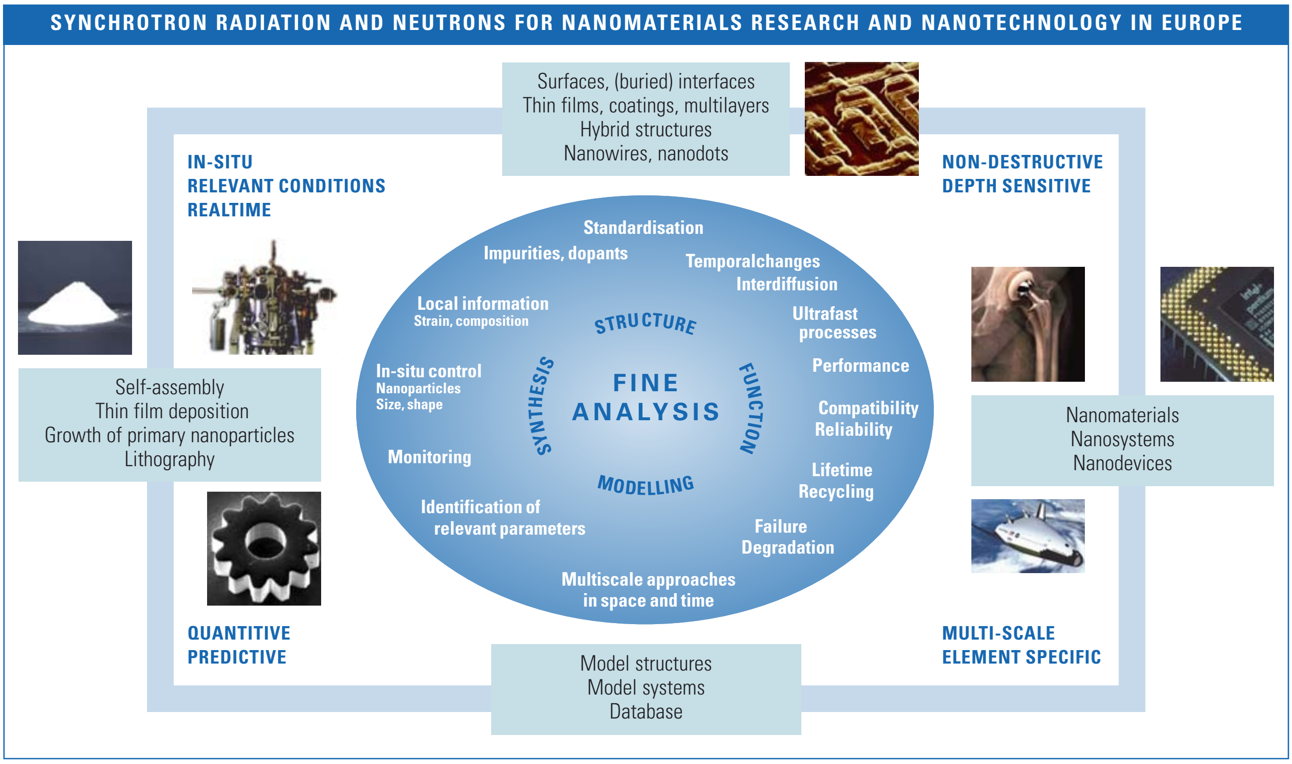

Fig. 8.4.1: Future need of synchrotron radiation and neutrons for nanomaterials development.

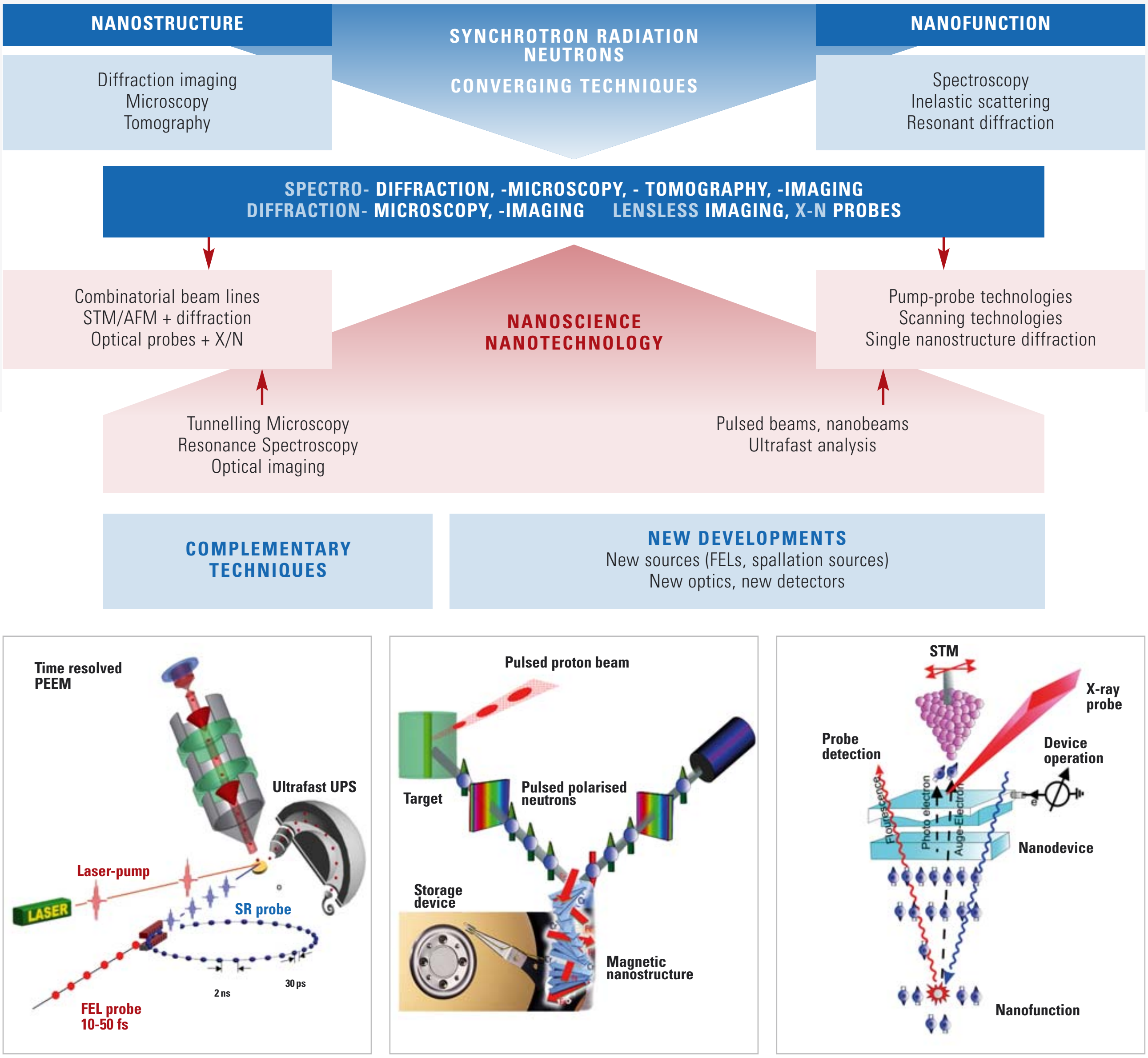

Fig. 8.4.2: Roadmap of synchrotron radiation and neutron probes for nanomaterials research.

In the past, synchrotron radiation and neutron facilities have been concentrating almost exclusively on the optimisation of the beam quality and on novel instrumentation. In the frame of GENNESYS, there will be an additional new focus on a specific selection of nanoscience topics. This is a rather unusual novel step for the European large-scale facilities which requires European coordination. This role should be taken over by the GENNESYS Council (see Chapter 11.11.).

9. IMPLICATIONS OF GENNESYS FOR EDUCATION

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The structure of our universities has changed little in the past fifty years, they are still organised in the traditional fields with little or no horizontal structures. In materials science – as in many other fields- much of the most exciting discovery potential is located at the boundaries between traditional disciplines: Already today, many new materials and devices are designed and developed by materials scientists working with chemists, physicists and engineers. It is thus apparent that we need to create new types of universities and colleges which have "departments without walls".

To face up to the massively sectorial investments of major or emerging countries targeting world leadership in some economic areas, Europe and partner institutions must overcome the fragmentation of the human and materials resources of European Research by gathering the best teams to share these resources through integrating them into new European organisations (GENNESYS European College of Excellence). The GENNESYS initiative represents a unique and attractive opportunity to gather and integrate geographically-dispersed human resources and effectively scientific facilities for training and promoting activities.

In order to compete with USA and Japan as well as China and India, Europe has to mobilise resources and establish Centres of Excellence in biology and nanomaterials research and education, as pioneered by our nuclear physicists and astronomers (CERN is a heroic example).

In nanotechnology, breakthroughs happen closer and closer to discoveries in basic research. In turn, the concept of "pre-competitive research" has little relevance for this field. Furthermore, progress in materials science and nanotechnology is to a large extent related to development of new characterisation methods.

Education challenge in nanomaterials science and technology

Many companies throughout Europe and the world report problems in recruiting the types of graduates they need, as many graduates lack the skills to work in a modern economy. For Europe to continue to compete alongside prestigious international institutions and programmes on nanomaterials, it is important to create a "European Elite College" which provides a top-level education and the relevant skills mix. This should be a new institution, involving new "satellites" of leading universities and other institutions throughout Europe. Such a college should cover education, training, sciences and technologies for research, and have strong involvement by European industry.

The elements for such a high level education are

- Multi-disciplinary skills;
- Top expertise in nanomaterials science & engineering;
- Literacy in complementary fields;
- Exposure to advanced research projects;
- Literacy in key technological aspects: exposure to real technological problems;

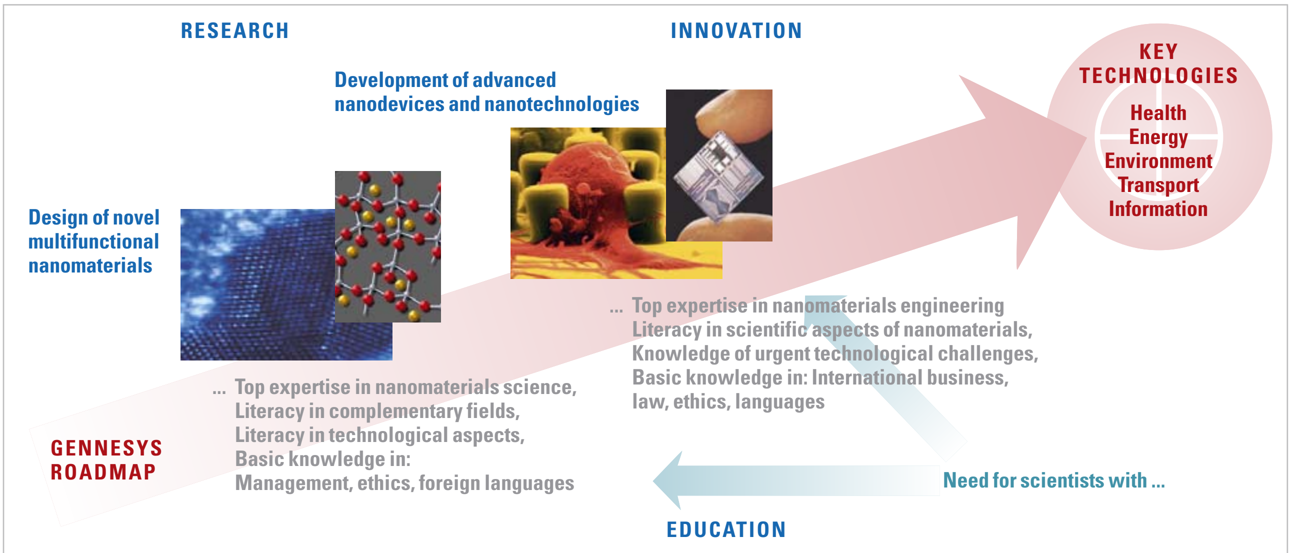

Fig. 9.1: The education challenge in nanomaterials science and technology.

- Basic knowledge in: social sciences, management, ethics, foreign languages;
- Literacy in neighbouring disciplines: international business, law, etc;
- Interlinkages between: education, research and industrial innovation: students will be ready for that research and development will provide;
- Sharing of post-docs, Masters and PhD students to foster the mobility of permanent researchers and professors between different institutions are needed to create "team spirit".

Companies, universities, governments, research organisations and technical societies must all strive to define their roles in this partnership.

The goal of the GENNESYS College is to develop a mechanism where education, research and industrial innovation merge. The GENNESYS vision is to create a place for training the most promising and highly motivated young scientists in Europe, where students will receive the highest standard of education and research management which will arm the graduates with the knowledge, methods and mechanisms to solve the future problems. The "output" will be graduate scientists and engineers excellently equipped for careers in top positions in the academic world, research management and industry to safeguard the future welfare of the society and meet industrial/economic challenges (see also Fig. 9.1).

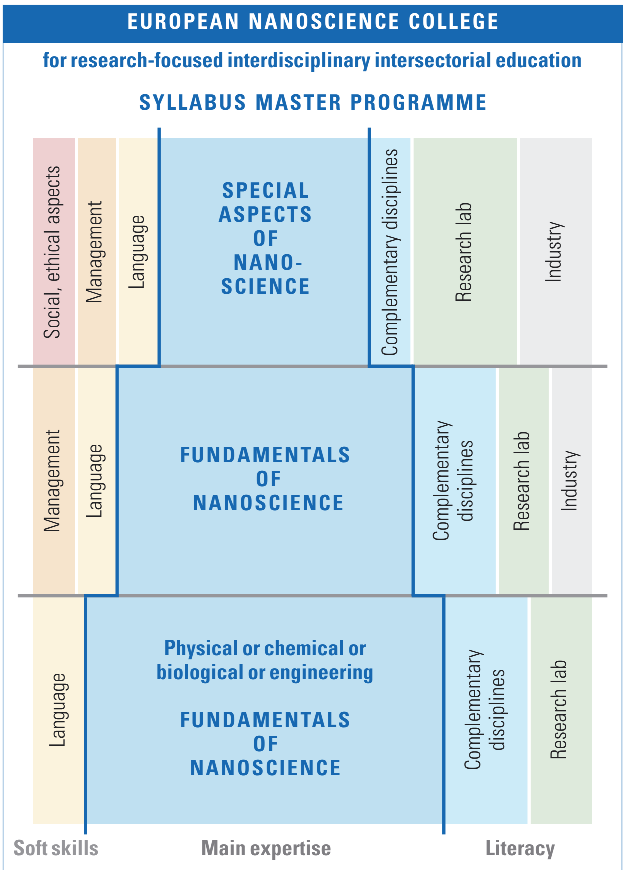

Fig. 9.2: New education syllabus for future materials scientists.

The new educational syllabus will be multi-disciplinary with an early involvement of the students in current research projects. The curriculum will be developed and adjusted jointly with industry. The studies are to be complemented inter alia with language, culture and society knowledge.

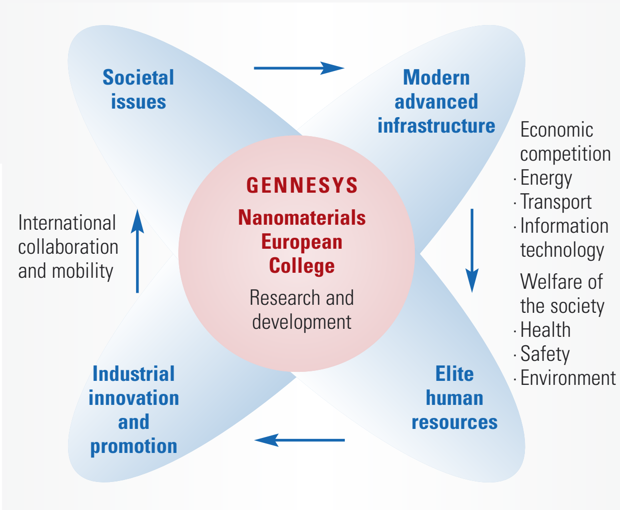

Fig. 9.3: GENNESYS COLLEGE: "Nanomaterials development scheme".

Partners of the European College

The international institute will offer both education and training. The training will cover master's degrees and professional doctorates, linking university researchers and training for industrialists with recognised qualifications.

The European College should have strong links with universities of excellence in Europe, nanomaterials research institutes, the research infrastructure and industry. The GENNESYS Centres of Excellence should play an important role.

The GENNESYS European College complements and supports the ideas of the European Institute of Technology. The GENNESYS European Nanomaterials College should become an influential body in Europe that stimulates, fosters and promotes education, research and innovation in nanomaterials, nanomaterials- related (life-sciences, physics, chemistry, engineering) science and technology in Europe. The college should become a platform which brings together different aspects of materials science in Europe and makes interfaces/synergetic interactions with all science-, science policy bodies and industry in Europe and worldwide. The structure could be envisaged as schematically represented by Fig. 9.5.

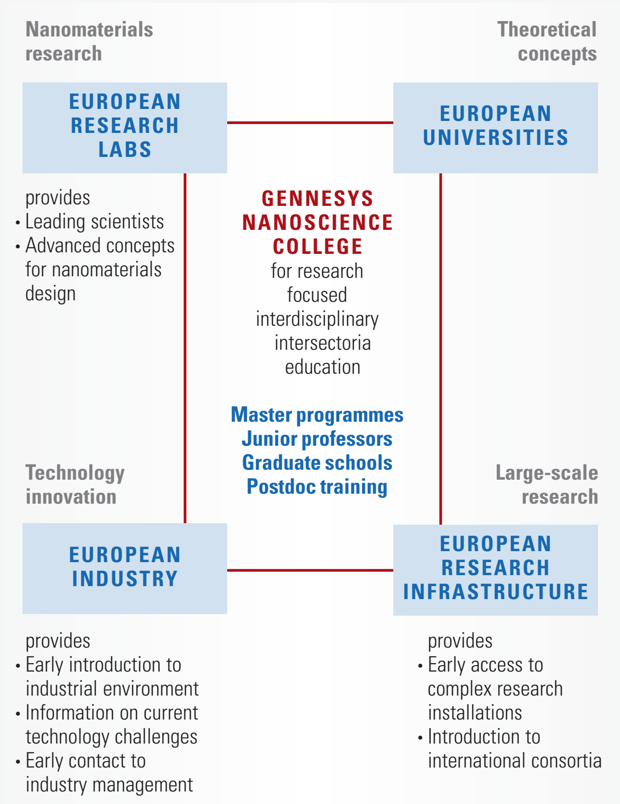

Fig. 9.4: Partners of the European Nanoscience College.

The benefits of a European Elite College in nanoscience are manifold:
The students will:

- Receive an excellence degree recognised across Europe and appreciated worldwide;
- Become attractive top-experts with literacy and management skills;
- Get promotion to leading positions in universities, research institutes, industry and government in Europe;
- Get early contact with key industrial problems.

The universities in Europe will:

- Join for an advanced international nanomaterials education;
- Attract the best students;
- Be able to offer joint academic appointments across disciplines, between universities and industries;
- Be able to offer new professional degree programmes with research institutes, the European research infrastructure and industry;
- Be involved in knowledge integration and transfer.

The Research institutes will:

- Be directly involved in focussing the education to the current research fields;
- Be able to recruit the best suited students.

Industry will:

- Be able to directly influence the skills mix of the students;
- Get in touch with the best talents facilitating their recruitment processes;

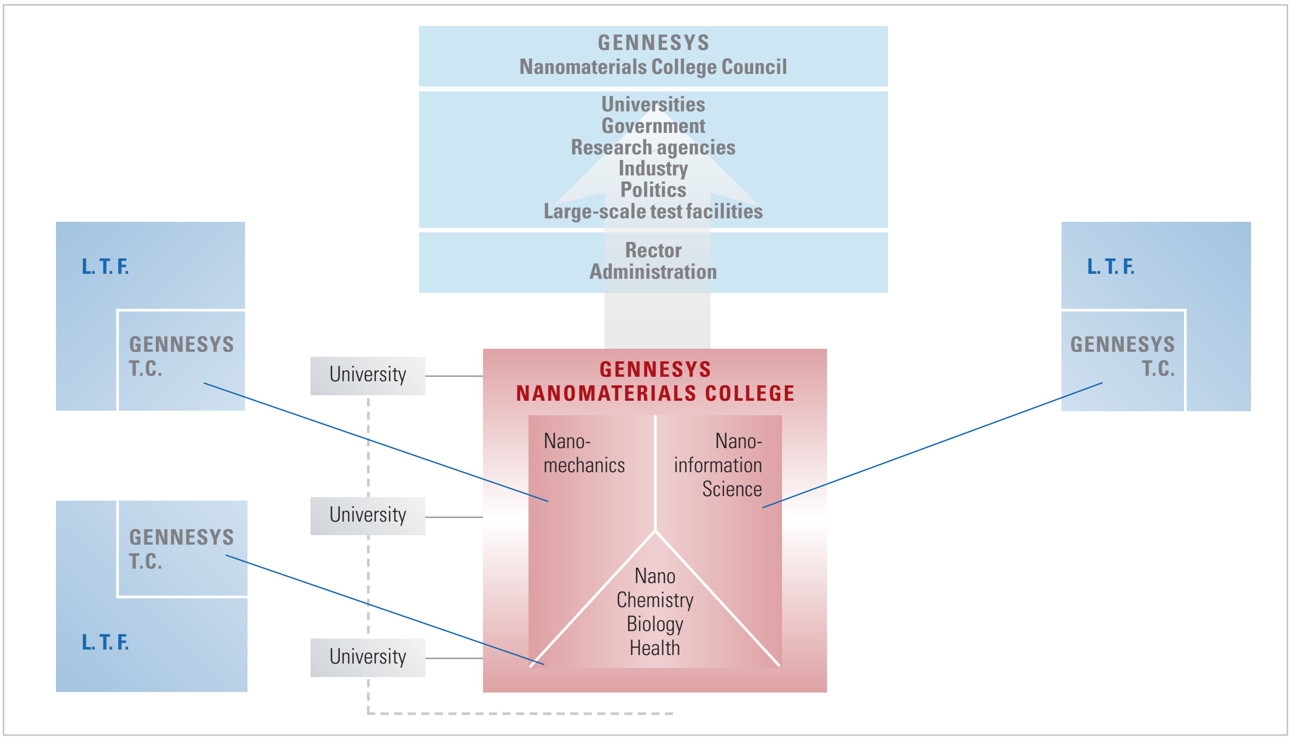

Fig. 9.5: GENNESYS College.

- Get in direct contact with scientific discoveries;
- Be able to help in the creation of spin-off companies.

The Society will:

- Benefit from a targeted education of young talented people;
- See more efficient scientists and engineers who tackle the urgent problems in energy, environment, health, and climate change.

Organisation and structure of the European College for Nanomaterials (see Chapter 11.12)

The education in nanomaterials science and technology demands excellent teaching staff and early access to the most advanced research laboratories and research infrastructures. The international institute for nanomaterials should operate under the sponsorship of the European Commission with the support from governments, European and national funding agencies and the research infrastructure. There should be a board of directors, an advisory board and the college rectorate. These boards should be represented by delegates from:

- Universities of excellence;
- Research institutions;
- Industrial research managers;
- Research infrastructure;
- Government bodies;
- Funding Agencies: national and European e.g. ESF;
- GENNESYS Centres of Excellence

Partnerships

Partnerships across disciplines and between universities, government laboratories and industry are crucial to leverage resources and strengthen interdisciplinary research, and to provide the awareness of technological drivers and potential applications.

The European Commission should provide incentives for the establishment of partnerships between universities, industrial labs and research centres and large-scale facilities that implement research in nanomaterials science.

These research and development partnerships should be encouraged in order to:

- Optimise the use of infrastructure and facilities;
- Enable cross-disciplinary research;
- Promote nanomaterials research in industry;
- Improve universities' and research labs' appreciation of industry priorities and needs;
- Develop integration mechanisms: to bridge the gaps between: education, research and industrial innovation; so that research discoveries spin-off into industrial applications;
- Share the risks and returns of long term research;
- Assemble teams that can recreate the fertile research environment of the former large industrial and governmental research labs;
- Develop the commercial exploitation and patenting of new technologies.

Conclusions

A European action plan in nanomaterials education has to be worked out urgently to underpin a sustainable nanomaterials research strategy. Strong efforts must be undertaken to improve integration of nanomaterials education and research, particularly at the boundaries of disciplines and to prepare flexible and adaptable nanomaterials scientists and engineers for the future.

A new framework of cooperation between universities, national research institutes and industry needs to be developed.

The proposed GENNESYS Nanomaterials European College" would ideally meet the requirements for the training of our future materials scientists and engineers. It would be a central institute with satellite schools at the GENNESYS "Centres of Excellence"– and with close associations to recognised research universities and corporate research in industry throughout Europe.

GENNESYS International Institute for Nanomaterials is ideally complementing the EIT (European institute for Innovation and Technology). Joining both institutions would become the motor for "Innovative Europe" in nanomaterials science and technology.

10. SOCIETAL, ETHICAL, ENVIRONMENTAL, AND HEALTH IMPLICATIONS OF NANOMATERIALS SCIENCE AND TECHNOLOGY

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[Affiliations chapter 12]

Since applications of nanotechnology will quickly penetrate all sectors of life and affect our social, economical, ethical and ecological activities, the general public's acceptance is compulsory for further developments of in the field of nanotechnology and its applications. This acceptance will be influenced by the low level of public awareness of many innovations in science, and especially, in nanotechnology. This is mainly due to the unpredictability of their properties at the nanoscale and the fragile public confidence in technological innovation and regulatory systems.

Consequently, it is of the utmost importance to educate the public, and to disseminate the results of nanotechnology development in an accurate and open way so that the general public will eventually accept nanotechnology.

In this endeavour, large international research and development organisations such as European synchrotron radiation and neutron facilities can be useful for:

- Educating people about science and technology; students, pupils;
- Informing the public about the benefits and risks of nanomaterials and nanoproducts;
- Evaluating, minimising, and eliminating risks associated with the manufacturing and use of nanomaterials and nanotechnology-enabled products (risk assessment);
- Exchanging with public authorities for the risk management of nanotechnology.

10.1. THE CHALLENGE OF A NEW FRONTIER

Historical aspects related to nanomaterials

Even through nanotechnology is a fairly new field, nanomaterials, however, are not:

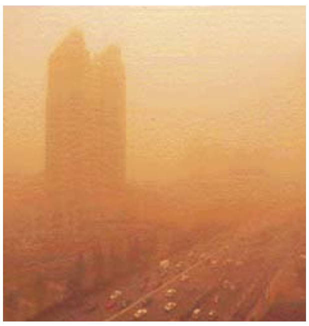
- 5000 years ago the Egyptians ingested gold nanoparticles for mental and body purification;
- Gold and silver nanoparticles were used in Persia in the 10th century BC in the manufacture of ceramic glazes, giving them a lustrous or iridescent effect. This technique was spread throughout most of Europe in the 14th century.

Nanoparticles are abundant in nature as they are produced in many natural processes, including photochemical reactions, volcanic eruptions, forest fires, and simple erosion, and by plants and animals, e.g. shedding of skin and hair (see Fig. 10.1.1). Though we usually associate air pollution with human activities – cars, industry and charcoal burning – natural events such as dust storms, volcanic eruptions and forest fires can produce such vast quantities of nanoparticulate matter, profoundly affecting air quality worldwide.

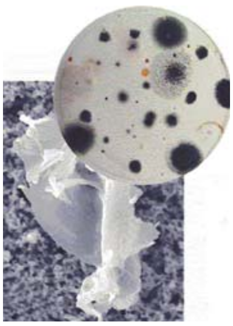
Nanosubstances can be generally classified as:

- Naturally occurring nanoparticles: e.g. virus, dust from desert, forest fire smoke;
- Ultrafine particles from established or as by-products of conventional current processes: e.g. Diesel exhaust particles, carbon black for photocopier toner;
- Engineered or structured nanomaterials: e.g. nanotubes, quantum dots.

NATURAL SOURCES OF NANOPARTICLES

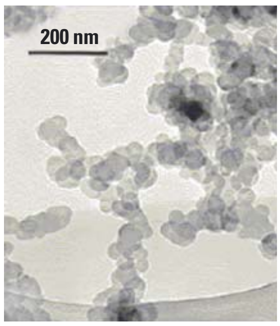


Beijing during a sand storm



Bacteria collected from African dust that reached North America

South California fires



TEM image of a smoke aggregate from a forest fire

Fig. 10.1.1: Nanoparticles in natural processes.

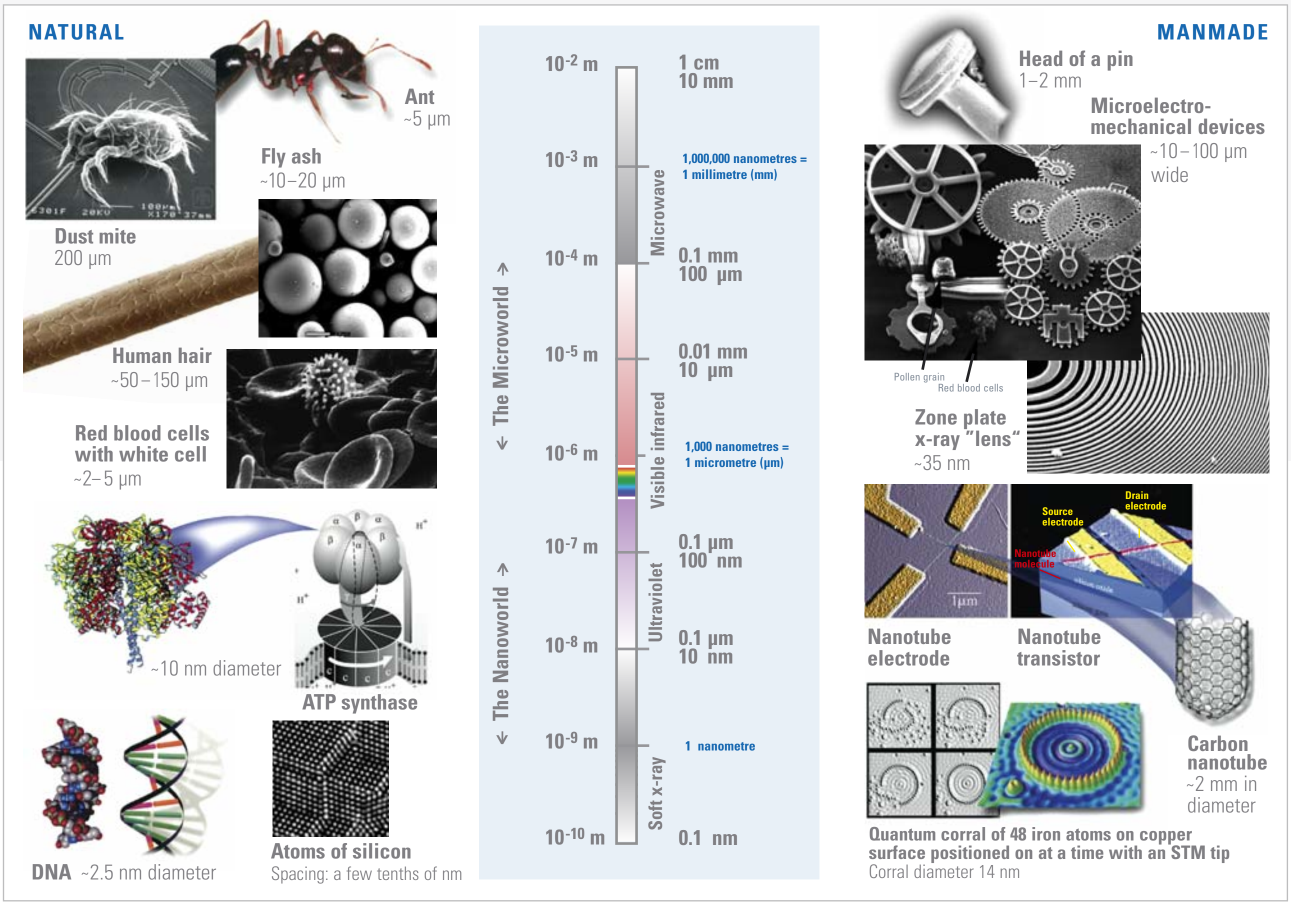


Fig. 10.1.2: Natural and manmade substances in function of length scales. Courtesy: Office of Basic Energy Sciences, U.S. Department of Energy.

Types of nanomaterials science and technology

Currently, new nanotechnology consumer products are coming on the market at a rate of three to four per week. The number of consumer products using nanotechnology inventoried by a US government agency grew from 200 in 2006 up to 600 in 2008. Health and fitness items, which include cosmetics and sunscreens, represent 60% of inventory products.

Nanoscale silver is the most commonly used nanomaterial in the consumer products using nanotechnology. Carbon, including carbon nanotubes and fullerenes, is the second highest nano-engineered material. Other nanoscale materials explicitly referenced in products are zinc, titanium (including their respective oxides), silica and gold.

A recent European investigation has defined a nanomaterial roadmap (Nanoroad 2015) that aims to identify the relevant nanomaterials with a high potential for future industrial applications. Seven main material categories were defined simply as: carbon-based materials, nanocomposites, metals and alloys, biological nanomaterials, nanopolymers, nanoglasses and nanoceramics.

These potential nanomaterials can be further classified into three main categories:

- **Evolutionary nanomaterials development:**
  This group can be defined as:
  - Historically larger technologies that have shrunk to the nanometre scale or
  - Improvements of existing products with nanomaterials.
  Typical areas of evolutionary nanotechnologies:
  - The semi-conductor technology has become a nanometre-scale technology;
  - Cosmetics have become a nanometre scale technology – nanoparticles in cosmetics and cosmetic systems.

- **Revolutionary nanomaterials science and technology:**
The discovery and innovation of new nanometre-scale products and technologies is highlighted here. A very specific discovery is the "carbon nanotubes" – Nanotube transistor.

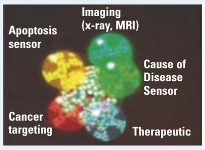
- **Natural nanomaterials science and technology:**
  - Functional- and structural nanometre-scale products formed on a natural base.

NATURAL SOURCES OF NANOPARTICLES

BENEFITS TO BIOMEDICINE AND HEALTHCARE

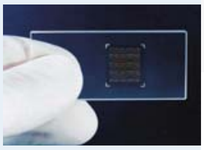
Gold nanoshells for cancer therapy

Biological nanodevices based on dendrimers:
- Recognise cancer cells;
- Diagnose the cause of cancer;
- Delivery of drug to target;
- Report the location of a tumor;
- Report the outcome of therapy (death of cancer cells).



Smart drug delivery

Lab-on-chips for: personalised drug development and molecular diagnostics, such as safety and timely bio-detection in order to avoid pandemics



Antimicrobial nanopowder and coatings

Gene transfection and therapy
Nucleic acid sequence and protein detection
Nanostructured materials for food packaging
- Layers with nanostructured materials will give reduced transport of oxygen and moisture from the air into the food, keeping it fresher for a longer period of time

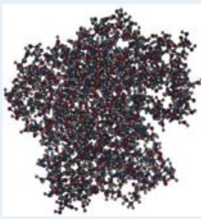
BENEFITS TO ENVIRONMENT

Elimination of pollutants:
- Automobile catalytic converters
- Power generation equipment

Water remediation:
- Removal of chlorine based solvents from contaminated water and soil

Conservation of resources

CO_2 and aerosol emission reduction



BENEFITS TO ENERGY

Low consumption MPU and memories

Low voltage display and TV

Low consumption lighting and signage

Efficient energy transmission:
- Nanowires, nanocoatings
- Self-cleaning nanomaterials for the removal of ice accumulation on power lines

High efficient energy batteries

High efficient photovoltaic cells
Hydrogen society:
- Production and storage of hydrogen
- Use of hydrogen in fuel cells for the production of electricity

Wind energy:
- Stronger and lighter wind turbine blades by adding carbon nanotubes in the regular composite materials

BENEFITS IN TRANSPORTATION

Nanocomposites:
- Lighter, stronger, heat-resistant parts of cars, planes, trains,...

Insulation materials:
- Porous and light-weight aerogels

Paints:
- Enhanced mechanical properties
- Scratch resistant

Self-cleaning windows

Car tires and bumpers

BENEFITS FOR MILITARY APPLICATIONS

Lighter, stronger heat-resistant armour and weapons

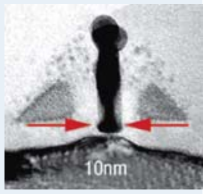
BENEFITS FOR INFORMATION TECHNOLOGY

Efficient, fast and cheap MPU
- Low cost processors and memories
- Quantum state logic & computing
- Bio-electronics

Wirelesss transmission:
- Increase in the data transmission rate

High density data storage:
- Spintronics
- Macromolecular memories

Flexible display:
- Organic electronics



BENEFITS FOR SAFETY & SECURITY

High sensitive and wireless sensors:
- Pressure-pipes,…
- Car pressure monitoring
- Gas for preventing any hazard
- Accelerometer: airbags,…
- Electrical resistivity
- Chemical activity
- Thermal conductivity

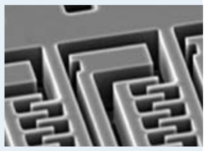


Table 10.2.1: Overview of nanomaterial benefits in multiple technologies

10.2. PROMISES, BENEFITS AND RISK PERCEPTIONS OF NANOMATERIALS SCIENCE AND TECHNOLOGY

The GENNESYS European nanomaterials science and technology initiative aims to fully realise the promise of nanomaterials science and technology and translate that promise into improvements in Europe's economy, security, and quality of life while at the same time protecting public health and environment.

Consumer's benefits of nanomaterials science and technology

Today, people unknowingly interact daily with various silicon micro- or nanoproducts: microprocessor units (MPU) and memory chips, pressure sensors, accelerometers, ink-jets for printers, micro-mirrors for display projectors are the most ubiquitous.

In the near future, the number of nanotechnology-enabled products introduced within society will certainly increase. Nanotechnology will be highly beneficial for consumers' benefits in various sectors of their daily life. Nanotechnology results promise benefits that will shift paradigms in many fields of research: biomedicine (imaging, diagnosis, treatment and prevention), environment (remediation and pollutants reduction), energy (conversion and storage), transportation, and information technology (computing, sensors and displays), as well as in safety and security (see Table 10.2.1).

Potential consumer risks related to nanotechnology

If the overall benefit of nanotechnology will be highly positive, concerns about societal, ethical, environmental and health implications have naturally arisen as nanotechnology has developed and as nanotechnology-enabled products have proliferated in the marketplace.

One big controversy related to the development of nanotechnology deals with the risks associated with its highly beneficial aspects. Two topics can be highlighted in this regard: (see also Table 10.2.2):

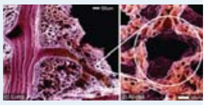
- **Privacy, safety and security:** Nanotechnology promises exponentially smaller and cheaper electrical components and sensors for equipment such as video cameras and computers. The same enhanced equipment that allows improving computational power can also be used to violate safety and security.

- **Health and environment:** Micro- and nanotechnologies usually employed nanoparticles or nanostructured materials. Fixed nanostructured materials, such as thin film coatings, microchip electronics and many other nano-engineered materials are known to be benign for living organisms. Uncontained nanoparticles, on the other hand, could represent a health threat, since they exhibit the ability to enter, and damage living organisms. Moreover, nanomaterials, as well as their by-products can be harmful to the environment: water, soil and the atmosphere. Nevertheless, some nanoparticles and nanomaterials could be highly beneficial to human health such as antioxidants, antibacterial/antifugal agents in various applications (air sanitizer sprays, pillows, vacuum cleaners, food storage containers and cellular phones), pollution elimination and/or prevention, and water remediation (see Table 10.2).

NANOTECHNOLOGY & NANOMATERIALS

POTENTIAL RISKS FOR HEALTH

Toxicology of engineered nanomaterials and by-product nanoparticles:
- Ability to enter into the human body
- Impact of biochemical processes



Harmful effects of "beneficial" nanomaterials ingested in the human body:
- Impact of nanoparticles used to destroy cancer cells on the whole of the human body
- Photochemical reactions of nanoparticles used in sunscreens and cosmetics

POTENTIAL RISKS FOR THE ENVIRONMENT

Toxicology of engineered nanomaterials and by-product nanoparticles:
- Accumulation and transportation in water, soil, and the atmosphere

Adverse impact of "beneficial" nanomaterials for the "food chain":
- Further impact of nanoparticles transported or transformed via micro-organisms such as bacteria and protozoa

POTENTIAL RISKS FOR SAFETY, SECURITY AND ETHICS

Invasion of privacy

Spread of spying sensors

Nanorobotics or other bio-nanotechnology ambitious applications

Table 10.2.2: Overview of the potential risks of nanomaterials.

10.3. SOCIO-ECONOMIC ASPECTS OF NANOTECHNOLOGY

Investment ideas

By 2010, annual growth of the markets for nanomaterials technology is expected to exceed 28%, or more than € 150 billion. This development will be attributed to expectations for improved quality of life, environmental concerns, energy savings and efficiency as well as security-related issues. Nanotechnology innovations are expected to provide lighter, stronger, safer and more efficient aircraft, cars, consumer electronics, new solar panels, batteries, super capacitors and fuel cell technologies and new classes of drugs, medical devices, cancer treatment, and biomaterials.

Nanotechnology highlights – a European view

Remaining competitive in a global market, securing energy supplies, guaranteeing personal security and meeting the environmental challenges of an industrial society are the main socio-economic driving forces for the future development of Europe's economy and well-being.

Nanomaterials are central to future breakthroughs within a range of industrial sectors, such as the chemical and petrochemical industries, pharmaceutical and medical companies, energy and transport sectors, metallurgy, information technology and personal security (see Fig.10.3.1). The enlarged European community provides potential for leading-edge development in the area of nanomaterials and nanotechnologies. Strong research groups, internationally pre-eminent industrial companies, and advanced neutron and synchrotron radiation facilities exist in Europe and form the foundations of a strong, knowledge-based society. The "intellectual property", i.e. the knowledge generated and expertise gained in GENNESYS will foster greater commercial exploitation (patents, spin-off companies,…), in turn making Europe more globally competitive, assuring our welfare.

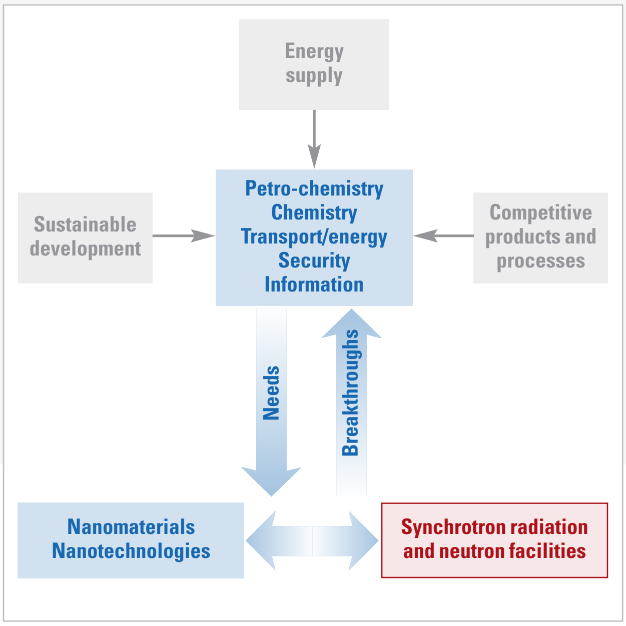


Fig. 10.3.1: The socio-economic perspective in relation to competiveness.

SOCIO-ECONOMIC REQUEST FOR EUROPEAN AERONAUTIC SYSTEMS			
Emission	Vision 2020 Estimated reduction	Influencing factor	
Noise	10 db	Airframe: Size/shape	Aero-engine
Fuel, CO_2	20 db	Airframe: Weight	Aero-engine
NO_x, Soot	30 db		Aero-engine

Fig. 10.3.2: Socio-economic requirements for European Aeronautic Systems (Vision 2020).

Socio-economic requirements in the transportation sector

- To achieve sustainable use of natural resources to protect the environment (as demonstrated by the emission reductions for aeronautic systems in Fig.10.3.2);
- To fulfill political demands such as the Kyoto Protocol;
- To develop advanced and intelligent transportation systems, enhanced passenger safety, end-user comfort and satisfaction.

Part of the socio-economic pressure on existing transportation systems evolves into technical demands which often require the development, processing, and characterisation of innovative material systems. Nanomaterials, either with nanosized morphologies or nanosized microstructural features, constitute some of the most promising recent innovations. Successful implementation of these nanoinnovations in transport systems requires the characterisation of materials and manufacturing processes by synchrotron/neutron scattering techniques (see Fig. 10.3.3).

10.4. SOCIETAL ACCEPTANCE OF NANOTECHNOLOGY

Risk management of nanotechnology is challenged by the enormous uncertainties about the risks, benefits, properties and future directions of nanotechnology applications. As nanotechnology has emerged from the laboratory into industrial manufacture and commercial distribution, the potential for human and environment exposure, and hence hazards with an associated risk, have become an increasing reality and priority. Risk management of nanotechnology is further challenged by the broad range of technology and products encompassed within the term "nanotechnology". Risk management of nanotechnology must take into account public perception about the potential risks and benefits of nanotechnology and the growing public demands for regulatory oversight. One must take into account that consumers react differently to various nanotechnologies: consumers are more negative towards some agrifood nanotechnology relative to non-food applications e.g. in the area of medicine. Japanese consumers have a much more positive attitude to the use of nanomaterials compared to Europeans.

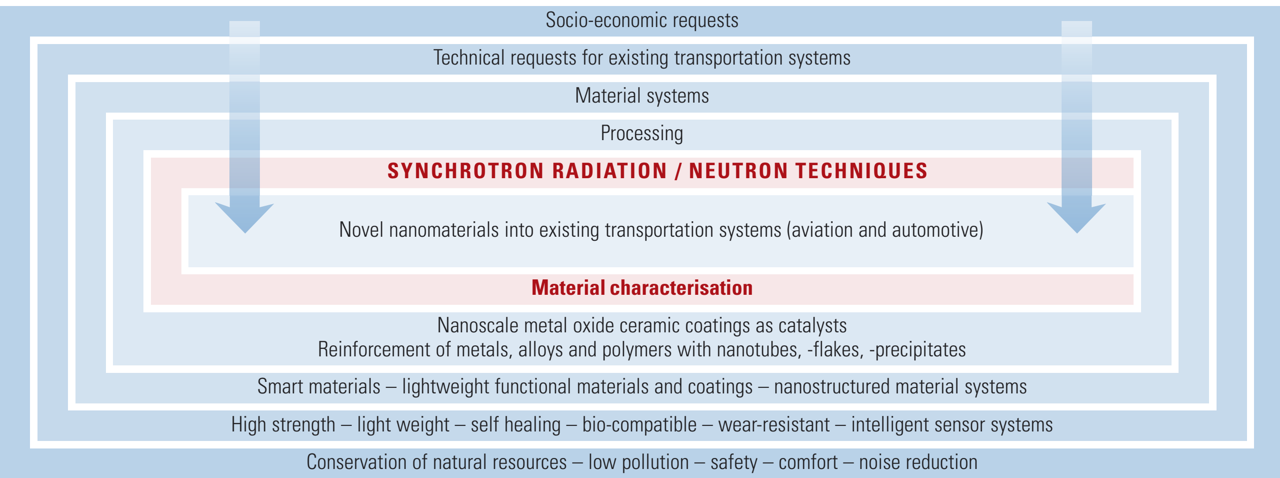


Fig. 10.3.3: Influences of socio-economic demands on the development of nanostructured materials for transportation systems.

Historical lessons learned

- Consumer values such as concern about the integrity of nature, and trust in regulatory systems influence societal and consumer acceptance;
- Assessment, management and communication of potential risks (and possibly benefits) associated with emerging applications of nanotechnology must be both transparent and societally inclusive;
- Novel risk-benefit assessment methodologies may be needed to evaluate; e.g. the health impact of nanotechnology;
- Risk (benefit) communication must address consumer concerns, and should not focus on non-technological estimates of risk alone;
- Individual consumer and citizen "control" over exposure to nanomaterials may be important, necessitating the implementation of effective traceability systems and associated information strategies;
- Lack of transparency in risk analysis systems and decision-making practices are not helpful in reassuring the public;
- First generation products which do not have direct benefits to consumers will militate against the development of positive societal attitudes;
- Order of entry into the market place is important - 1st generation products with tangible and desirable consumer benefits will facilitate positive attitudes towards nanotechnology applications more generally.

Role of public engagement (Fig. 10.4.1)

Involving the public in the debate about nanomaterial development, application and regulation may facilitate public acceptance as citizen's concerns and preferences can be identified and discussed.

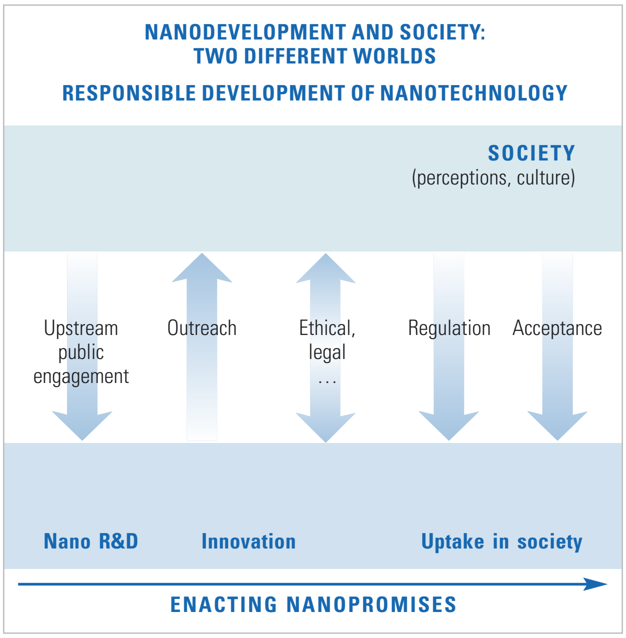


Fig. 10.4.1: Flow diagramme showing the acceptance stages for nanomaterials.

In order to be successful, public engagement exercises need to be proactive (i.e. conducted before public attitudes have crystallised) and have political impact. Some challenges associated with informal discussion include:

- Critical: demonstrable facts are distinguished from beliefs;
- Thoughtful: discussion leads to creative solutions.

Consumer acceptance of nanotechnology

One of the greatest challenges facing nanotechnology is confronting the current lack of public understanding of the underlying science. Communicating research results on the assessment, minimisation and prevention of nanotechnology risks and benefits outside the scientific community is also challenging, but it is essential for its development in order to prevent misunderstanding of the nanotechnology industry.

- Education of the general public about science and nanotechnology: This education can be envisioned either at grade-school or at college. Teaching children about nanotechnology is a great tool to indirectly inform the general public as well.
- Information of the general public about the benefits, risks and probabilities associated with nanotechnology:
  Dissemination of information to the public must be transparent, reliable and performed by all participating actors: stakeholders, including public interest groups, the scientific community, nanotechnology manufacturers and public authorities (see Fig. 10.4.1). Communication should address all the aspects related to ethics, integrity of nature, risk-benefit assessment methodologies and regulatory systems across different social, cultural and demographic groups.
- Global understanding of nanotechnology specific risks and benefits: This is fundamental for the consumer if large and small industries are to operate on a level playing field, and developing economies are not to be denied essential information about safe nanotechnologies

Environmental safety and health acceptance of nanomaterials

The production, use and disposal of nanomaterials will inevitably lead to their appearance in the air, water, soils or organisms. The intentional and unintentional release of nanoparticles and nanomaterials may consequently impact long-term phenomena such as climate change, ore and petroleum deposition, paleomagnetism and ground water composition.

Currently, the lack of reliable and accurate technical data on the topic provides fertile ground for both nanotechnology proponents and sceptics to make contradictory and sweeping conclusions about the safety of engineered particles for human health and ecosystems. It is therefore imperative to carry out investigations devoted to the development of a comprehensive understanding of the properties, interaction, and fate of natural and anthropogenic nanoscale and nanoengineered materials in human health and environment.

Measurement science and technology should be developed in order to:

- Identify conditions for safe manufacturing, use and disposal of nanomaterials;
- Understand how the morphology, size, composition, surface reactivity, agglomeration, kinetics and transport of nanoparticles (nanotoxicity) affect the human health and environment, including climate change;
- Investigate the kinetics and biochemical interactions of nanoparticles with organisms;
- Study nanoparticle aging: surface modifications and change in aggregation state after interaction with bystander substances in the environment with biomolecules and other chemical systems.

In order to assess the safety of complex multi-component and multifunctional nanomaterials, scientists will need systems capable of predicting the potential impact of new nanomaterials, devices and products.

The challenge is three-fold:

- Develop validated models for predicting the release, transport, transformation, accumulation and uptake of engineered nanomaterials in the environment;
- Develop models for predicting the behaviour of engineered nanomaterials in the human body, including dose, transport, clearance, accumulation, transformation and response;
- Use predictive models for engineering nanomaterials that are safe by design

These models should:

- Relate the physical and chemical properties of nanomaterials;
- Allow an integrated approach for predicting potential impact of engineered nanomaterials and nanoproducts;
- Estimate impact within susceptible populations

Developing robust ways of evaluating the potential impact – good or bad – of a nanoproduct from its initial manufacture and use to its ultimate disposal, must engage both scientific and policy communities (see Fig. 10.4.2).

Risk governance of nanotechnology
Relevant existing regulatory standards for safety

- Responsible scientists need to debate both positive and negative aspects of nanomaterials science and technology transparently and in full view of the public. Such debates will "rule" on benefits and risks of nanomaterials science and technology, and such a process is an important step towards entering into public debate about new technologies.

- European and national regulatory mechanisms are in place for assessing and regulating workplace, environmental, and health risks of new technology materials:
  - Food and food packaging; food additives, pharmaceuticals to be metabolised by the human body;
  - Diagnostic or therapeutic medical devices;
  - Substances incorporated into consumer products

- Active efforts are underway to ensure that these regulatory mechanisms or appropriately amended ones provide proper coverage of nanotechnology – based materials.

Strategies for improving governance practices associated with nanotechnologies

Many important emerging issues are linked to the development of effective governance practices. Key issues include the:

- Development of societally acceptable procedures for testing the toxicity of nanotechnology-based materials and products;

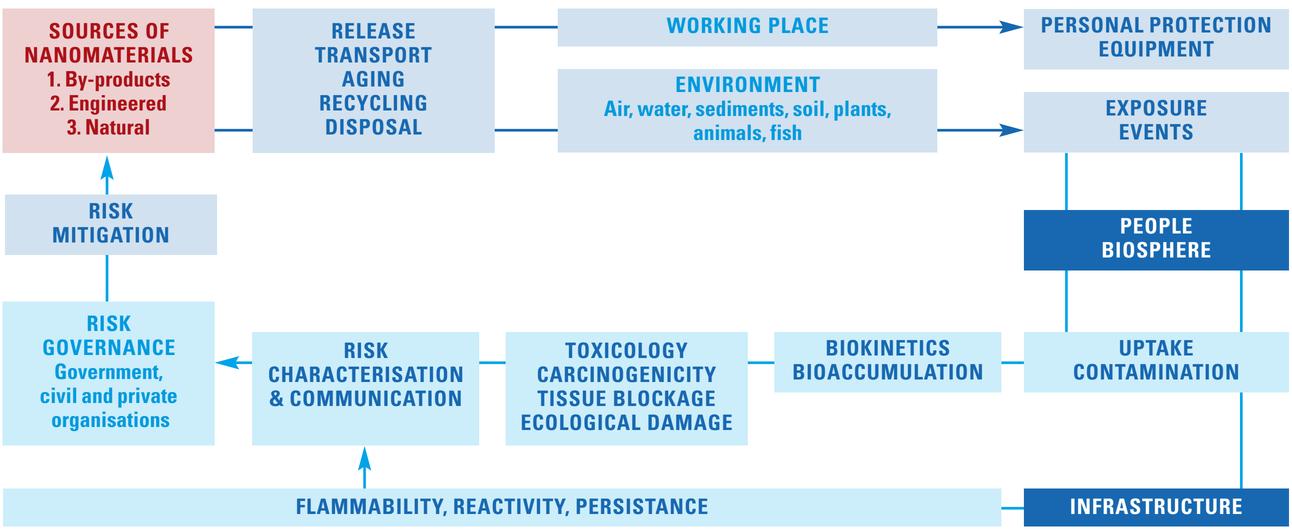


Fig. 10.4.2: Environment, safety and health research and regulatory for nanomaterials.

- Identification of the implications of risk and benefit associated with different nanotechnology applications for optimising transparent governance practices;
- Development of effective mechanisms for incorporating the views of stakeholders (including the public) in governance practices.

10.5. ROLE OF LARGE SYNCHROTRON RADIATION AND NEUTRON FACILITIES

Synchrotron radiation and neutron based tools open new perspectives at the intersecting frontiers of materials science, biology, medicine, physics, chemistry, engineering and geological sciences. In order to cope with the increasing pace of nanotechnology development, synchrotron radiation and neutron performance should be improved in order to enable:

- Imaging and characterisation of nanomaterials and nano-enabled products at the atomic scale;
- Measurement into various dynamic ranges; from attoseconds to milliseconds;
- In-situ, in-vitro and in-vivo measurements;
- 3-D measurements at the tens of nanometre scale for the analysis of nanodevices;
- Full analysis of nanomaterial and nanodevices using combined analyses.

These investigations are increasingly important for assessing benefits/risks, and preventing the associated risks related to any nanomaterial or any nanotechnology-enabled product. Since x-rays and neutrons allow for the characterisation of matter in all its phases using non-destructive, in-situ and in-vivo methods with high dynamics, synchrotron radiation and neutron facilities are perfectly suited for investigating, understanding and predicting the behaviour of engineered nanomaterials in the environment, including contributions to climate change, and in the human health as a function of their:

- Structural parameters: morphology, size, composition, surface reactivity, agglomeration;
- Kinetics, biochemical reactions with cells and organisms , short- and long-term toxicity;
- Transport, location, accumulation;
- Aging: surface modification, aggregation state, interaction with biomolecules and other chemicals.

For predicting the materials´ impact on the human health and the environment, x-ray- and neutron-based instruments should be used for:

- Measuring structural parameters of individual and assemblies of nanoparticles, nanocomposites and molecules;
- Determining elemental composition and bonding states at surfaces;
- Direct probing of catalytic activity of nanomaterials;

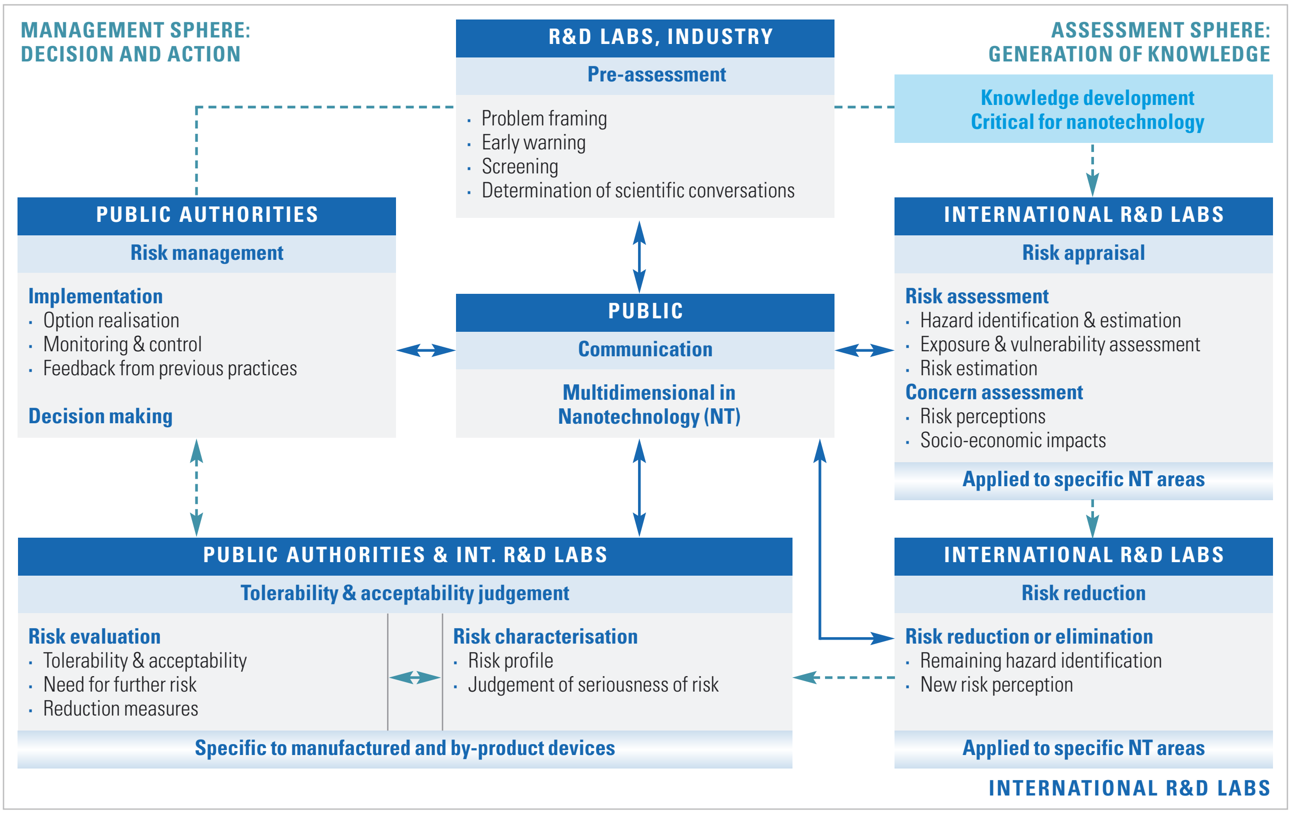


Fig. 10.5.1: Risk assessment and management framework for nanotechnology (NT).

- Investigating the dynamics of the interactions between nanomaterials with the human body and the environment;
- Characterising the structure and dynamics of adsorbed species, reaction intermediates, biological and chemical products

European synchrotron and neutron facilities must contribute in the education of the general public about nanoscience and nanotechnology, and in disseminating information about the research results concerning the assessment, prevention and elimination of risks, and about benefits of nanomaterials, devices and products (see Fig. 10.5.1).

The enlarged European community has the potential for leading-edge development in the area of nanomaterials and nanotechnologies. Strong research groups, internationally pre-eminent industrial companies, and advanced neutron and synchrotron radiation facilities exist in Europe and form the foundations of a strong knowledge-based society, in turn making Europe more globally competitive, assuring our welfare.

10.6. CONCLUSIONS – FUTURE RESEARCH – MAJOR CHALLENGES

Development of a nanomaterials science and technology strategy related to environment, health and safety

- Support research in order to safely develop and apply nanomaterials technology for societal benefit and economic growth in parallel with research to protect public health and environment in an improved way;
- Aim to maximise benefits while developing an understanding of potential risks and the means to manage such risks;
- Research equally informed by research and information needs of agencies with regulatory and oversight responsibilities;
- Collaborate on European and international base: share data, develop standard materials, agree on testing protocols.

European research programmes

- Identify, understand and minimise the risks associated with the development of nanomaterials and products;
- Analysing the life-cycles of nanomaterials used in the Flagship to identify where humans and the environment may be at risk from exposure;
- Monitoring workshop exposures to nanomaterials;
- Determining the impact on human health upon workplace exposure and from use of products containing nanomaterials;
- Determining nanomaterial's toxicity to the ecosystem in soil and water;
- Fully characterising the properties of nanomaterials and determining the nanoparticle matrix associated with any toxic effect;
- Develop a set of human and environmental predictive models for the toxicological effects of nanomaterials;
- Initial focus on metal oxides and carbon nanotubes.

Societal acceptance of nanomaterials and their commercialisation

The above is dependent on the following factors:

- Education of the public in science and technology;
- Effective governance;
- Transparent, frequent and accurate communication to the public of understandable information by all participating actors; from academic researchers and manufacturers to government agencies;
- Tangible societal and consumer benefits;
- Societal inclusivity in regulation and product development.

Role of synchrotron radiation and neutron facilities

In order to have a sound understanding of all the different nano-phenomena taking place, the availability of advanced analytical and structural techniques is vital. In addition to conventional techniques, synchrotron radiation and neutrons can offer great benefits to society in directing the nanotechnology developments such as through the study of in-situ, in-vivo and in-vitro processes, many of which can be studied non-destructively. These advanced experimental techniques may offer many benefits in nano-industry, and are ideal techniques to create the necessary knowledge base.

Since European synchrotron radiation and neutron facilities are operating in an international environment, they are also ideally suited for disseminating transparent information about the benefits, hazards and risks of nanomaterials and nanodevices from their initial manufacturing step and use to their final disposal.

European strategy and research programme

One of the important steps in the promotion of nanomaterials and nanotechnologies to the public is to ensure that there is adequate explanation and understanding of the benefits e.g. welfare and health and the hazards e.g. toxicology that nanomaterials and technologies can bring; coupled with an understanding of the basic science and engineering which is used in the production, processing and applications of nanomaterials and associated technologies.

A European research programme should be initiated to define the actions necessary to ensure public acceptance of nanomaterials. This programme should have both a physical sciences and a social sciences approach (see Fig.10.6.1). It should gather social researchers, R&D laboratories and private partners involved in nanomaterials, stakeholders and some components of the general public for:

- Defining general scientific education requirements for a better understanding of nano-enabled products;
- Highlighting benefits and potential risks associated to the manufacturing, use and disposal of nanomaterials and nano-enabled devices;
- Widely disseminating the results about the toxicology and bio-compliance of engineered and natural nanomaterials and nano-enabled

products and their potential impact on the human health, the bioenvironment, the ethics and the quality of life;

- Proposing some specific guidelines for a better risk management of nanomaterials and nano-enabled products from the risk assessment investigations performed by independent laboratories such as large-scale neutron and synchrotron x-ray facilities

Neutron and synchrotron x-ray methods should be introduced as advanced and unique scientific techniques, which have been applied for many decades to the study of problems that have applications in biology, pharmaceuticals, engineering and electronics. They are mandatory to generate the information that is required for the safe and sustainable use of natural and engineered nanomaterials in consumer applications.

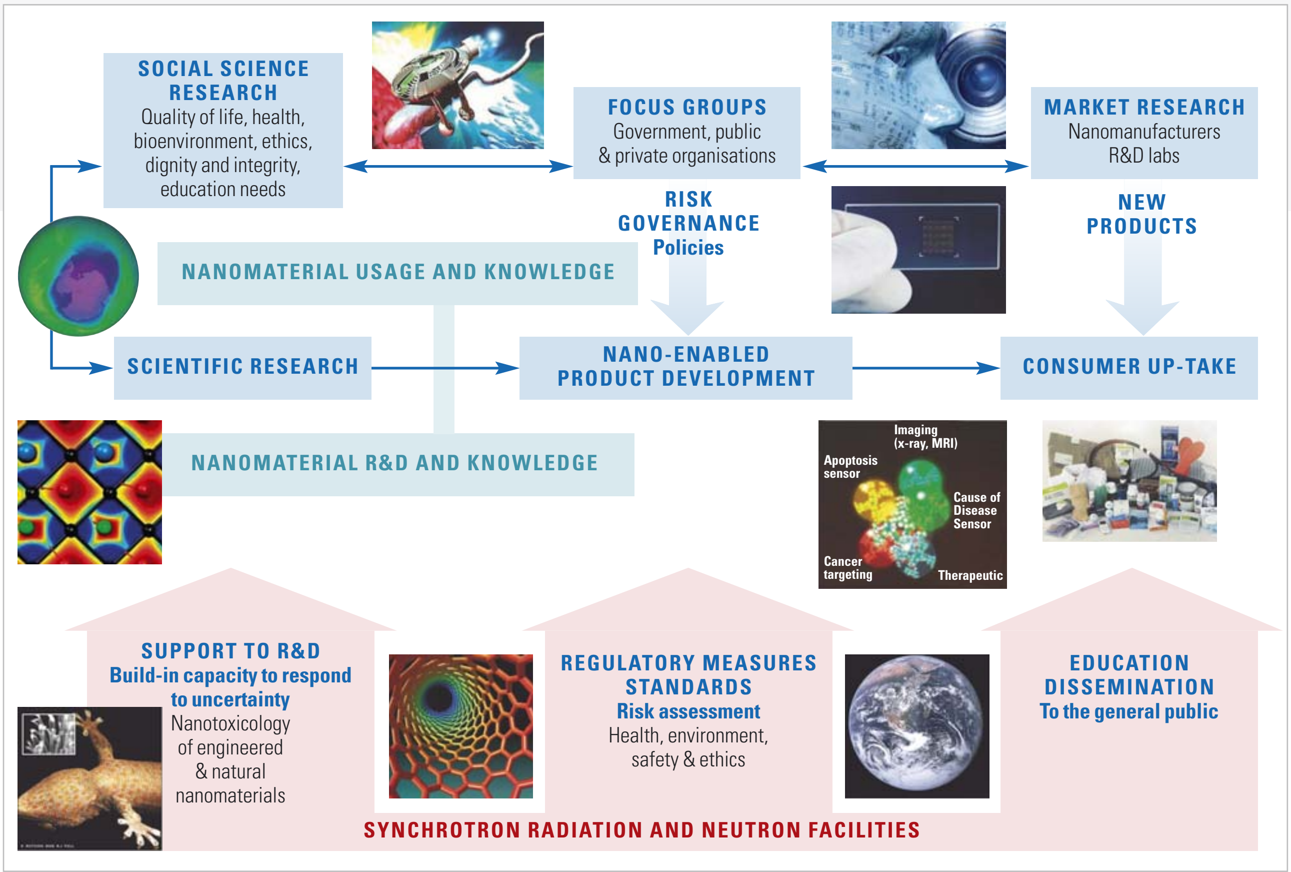


Fig. 10.6.1: Role of synchrotron radiation and neutron facilities in research and development and the manufacturing of a nanotechnology-enabled product.

11. CONCLUSIONS – RECOMMENDATIONS – FUTURE STRATEGIES AND ACTION PLAN

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11.1. OVERALL CONCLUSIONS: BARRIERS AND GENERIC CHALLENGES

The future welfare of the European citizen depends intimately on innovations in so-called key technologies encompassing information and communication, energy and environment, health and transport. Today, it is common wisdom that these innovations require, in turn, novel, made-to-measure nanomaterial structures which can: process data at a speed of terabytes per second; safely store the data in the smallest dimensions; assure biocompatible transplants; remove monoxides in modern car catalyzers; efficiently separate protons and electrons in fuel cell technology and electrons and holes in novel organic solar cells; and which can withstand – with a minimum weight – the highest mechanical and thermal loads. A paradigmatic example is taken from the IT roadmap which aims for smaller and faster material structures and improved data storage – it strives for $10nm^2$ small structures to store 1 bit (enabling a storage density of 5 Terabit/in^2). Europe has a superb track record in the development of novel materials and new material phenomena: high-T_c superconductors, the quantum Hall effect, the giant magnetoresistance effect which revolutionised hard disc data storage, the C_{60} chemistry, the development of the scanning tunneling microscopy and the miscroscopic investigations of chemical reactions at catalytic surfaces which opened the gateway to the molecular understanding of heterogeneous catalysis. These are only a few heroic examples of the many recent achievements in materials science which show that Europe's brains are top class. However, in order to be competitive in the future advancement of nanomaterials science and development of nanotechnology with the US and Japan, Europe needs improved research and funding strategies.

Modern materials science depends on several interdisciplinary elements: the materials range from metals, ceramics and semiconductors to polymers, organic and biomaterials which are brought together on the nanoscale to create new functions by solid state physicists, chemists and biologists who work together and stay in close contact with industrial research labs. Experts in atom-controlled material synthesis, in the advanced microsopic analysis of the materials and in the modelling of materials have to interact in an intimate way. Modern synthesis, analysis and modelling of materials often require large and expensive facilities; fragmented efforts often lead to costly and ineffective local solutions.

The GENNESYS foresight study has investigated in detail the state of the art, future opportunities and challenges in this super-disciplinary development of nanoscience and nanotechnology. It has put together recommendations as to how to overcome fragmentation of efforts and to develop novel research strategies with the existing European research infrastructure, i.e. with the modern synchrotron radiation and neutron facilities which hold an enormous analytical potential to interrogate nanostructures and nanofunctions and to monitor nanophenomena under environmentally and industrially relevant conditions.

Novel analytical technologies exploiting the unique properties of synchrotron radiation and neutrons in order to access nanostructures and nanofunctions in deeply buried material architectures and under relevant external conditions, will play a crucial role in providing key structural and dynamical information that will pave the way to innovations in nanoscience and nanostructured materials. This will finally lead to the control of nanoscale architectures, design and application. These analytical technologies which have been developed and are still being developed at synchrotron and neutron centres must be exploited more efficiently in a new European nanoscience action plan. Revolutionary new analytical concepts which will be based on accelerator-based x-ray and neutron radiation (i.e. free electron lasers and spallation neutrons) must already be implemented in a sustainable European nanoscience concept.

First year of volume production	2003	2005	2007	2009	2011
Technology generation (half pitch, 1:1, printed in resist)	90 nm	65 nm	45 nm	32 nm	22 nm
Isolated lines (in resist) [Physical gate, metallised]	53 nm [37 nm]	35 nm [25 nm]	25 nm [18 nm]	25 nm [13 nm]	13 nm [9 nm]
Chip frequency	2.5 GHz	4.9 GHz	9.5 GHz	19 GHz	36 GHz
Transistors per chip (HV) (3x for HP; 5 for ASICs)	190 M	390 M	770 M	1.5 B	3.1 B
DRAM memory (bits per chip)	1.1 G	2.2 G	4.3 G	8.6 G	34 G

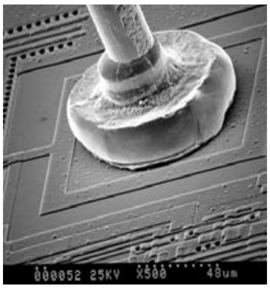


Fig. 11.1.1: Data taken from the IT roadmap.

Although the established nanotools for structural and dynamic investigations of nanostructures and nanomaterials, such as transmission electron microscopy, scanning surface probes, nuclear magnetic resonance, or optical spectroscopy, will retain their importance for solving nanoscale problems, advanced neutrons and synchrotron radiation experiments must in future provide advanced nano-information which are otherwise inaccessible. These key contributions of synchrotron radiation- and neutron-based techniques are during in-situ investigations under relevant environments and in the non-destructive interrogation of buried nanostructures and nanofunctions. Many applications will depend on emerging many-body phenomena, requiring characterisation of the spatial and temporal correlations between various components, and thus demanding a versatile spectrum of advanced and dedicated analytical techniques. Both synchrotron radiation and neutrons cover all relevant length scales relevant in nanoscience, from the atomic structure of individual building blocks to assembled functional structures. At the same time, synchrotron radiation- and neutron-based spectroscopy techniques allow the dynamic response to be determined over a wide range of timescales ranging from ultrafast structural relaxation to slow diffusion processes. Furthermore, the data analysis is generally based on rigorous and robust theories which allow straightforward and unambiguous interpretation of the data. The subtle differences in the coupling of x-rays and neutrons to matter must be further exploited to broaden the range of applications in a truly complementary fashion. It is thus clear that the quality of the further development of nanoscience and nanotechnology in Europe will depend strongly upon the availability of such advanced analytical techniques which are provided by the European large-scale facilities.

The future challenges for the large-scale facilities are to meet these challenges in nanomaterials science and nanotechnology. There is a need for appropriate upgrading of the sources, for the development of new sophisticated instrumentation, for the convergence of analytical approaches, and particularly for the creation of dedicated and well-equipped pre- and post-exposure laboratories run by cross-disciplinary research consortia on site, as well as for new access schemes, flexible onsite support and for efficient data analysis concepts adapted to untrained materials scientists and industry. This GENNESYS foresight study outlines areas for research and development, where synchrotron radiation- and neutron-based techniques should be developed to meet the nanomaterials challenge for the 21st century.

Materials design of tomorrow will increasingly be done by the control of individual atoms, ions and molecules. This poses serious challenges in the synthesis and analysis on three different levels: (i) generic challenges which are associated with the nanosized objects, (ii) material-specific challenges which are intimately related to chemical bonding and (iii) technological challenges which are concerned inter alia with the performance, quality assurance and degradation of real nanodevices (Fig. 11.1.2).

The GENNESYS foresight study has collected the input from more than 500 experts:

- A detailed account on the findings (state of the art, future needs and challenges), conclusions and recommendations are discussed in the Chapters 2 – 10.
- The key conclusions and recommendations are summarised in this chapter, in the associated Subchapters 11.2. – 11.9.

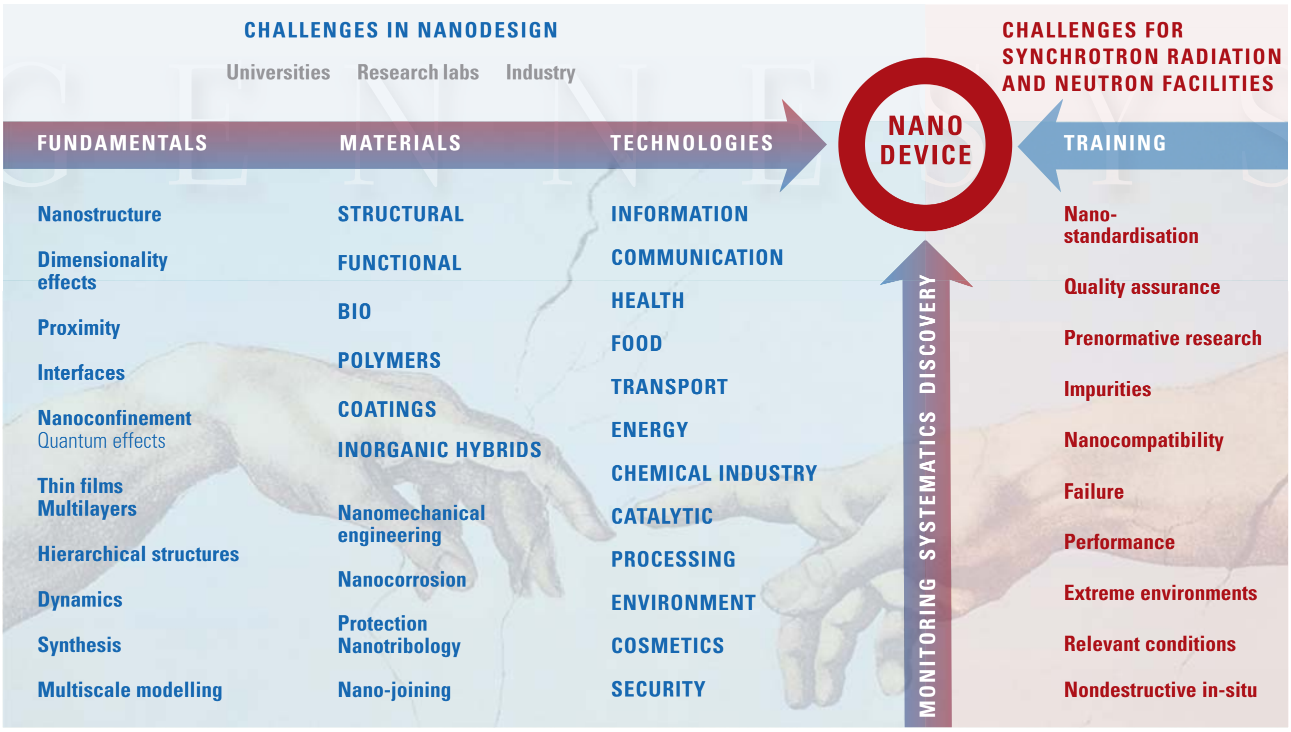


Fig. 11.1.2: Objective of the GENNESYS foresight study.

11.2. KEY CHALLENGES FOR FUNDAMENTAL RESEARCH

Progress in the development of nanoscience and nanotechnology can only be achieved through strong efforts in fundamental research. The key challenges are in: (i) the precision synthesis of novel nanomaterials with new functions; (ii) the design of new nanostructures which exploit the entire toolkit of the nanospace to evoke new properties and functions by tuning interactions, nanoconfinement geometries and proximity effects; and in (iii) multi-scale modelling.

Most of these challenges are generic to the nanodimensions and have to be solved for all classes of materials. The main goals of this fundamental effort are to:

- Conceive and design new nanomaterials and nanostructures;
- Probe their stability under increasingly advanced technological conditions;
- Discover new properties and functions;
- Test/upgrade them for/to technological relevance.

The controlled synthesis of nanomaterials and nanostructures, the microscopic control of their size, shape and structure and the associated nanofunctions require a new degree of analytical knowledge and technologies to be implemented in the academic and industrial research strategies which are generically related to the small size of the nanostructures. An intimate handshake between experts in synthesis, advanced analytical tools and nanomaterial modelling is a prerequisite for success. A strongly increasing need for tailored analytical technologies in nanoscience is predicted for the next 10 to 15 years, thus it is mandatory that the synchrotron radiation and neutron facility operators adjust and open their unique analytical potential to this European effort (see Fig. 11.2.1).

11.2.1. ROADMAP FOR FUNDAMENTAL RESEARCH IN NANOMATERIALS SCIENCE

Fundamental research in nanoscience encompasses a wide area of interdisciplinary activities with the goal to create further knowledge. The milestones of this endeavour are shown in the roadmap in Fig. 11.2.2. The ambitious goals laid down in the roadmap "Fundamental research in nanomaterials science" require an enhanced effort in fundamental research which joins the efforts from academia, research labs, industry and the European research infrastructure. The key areas are:

- **On-line control of precision synthesis of nanoparticles and nanostructures**

  Reproducible processing of nanostructured materials requires the detailed understanding of the relationship between processing conditions and resulting nanostructures and their properties. The ultimate goal is to develop guidelines for the synthesis of nanoparticles

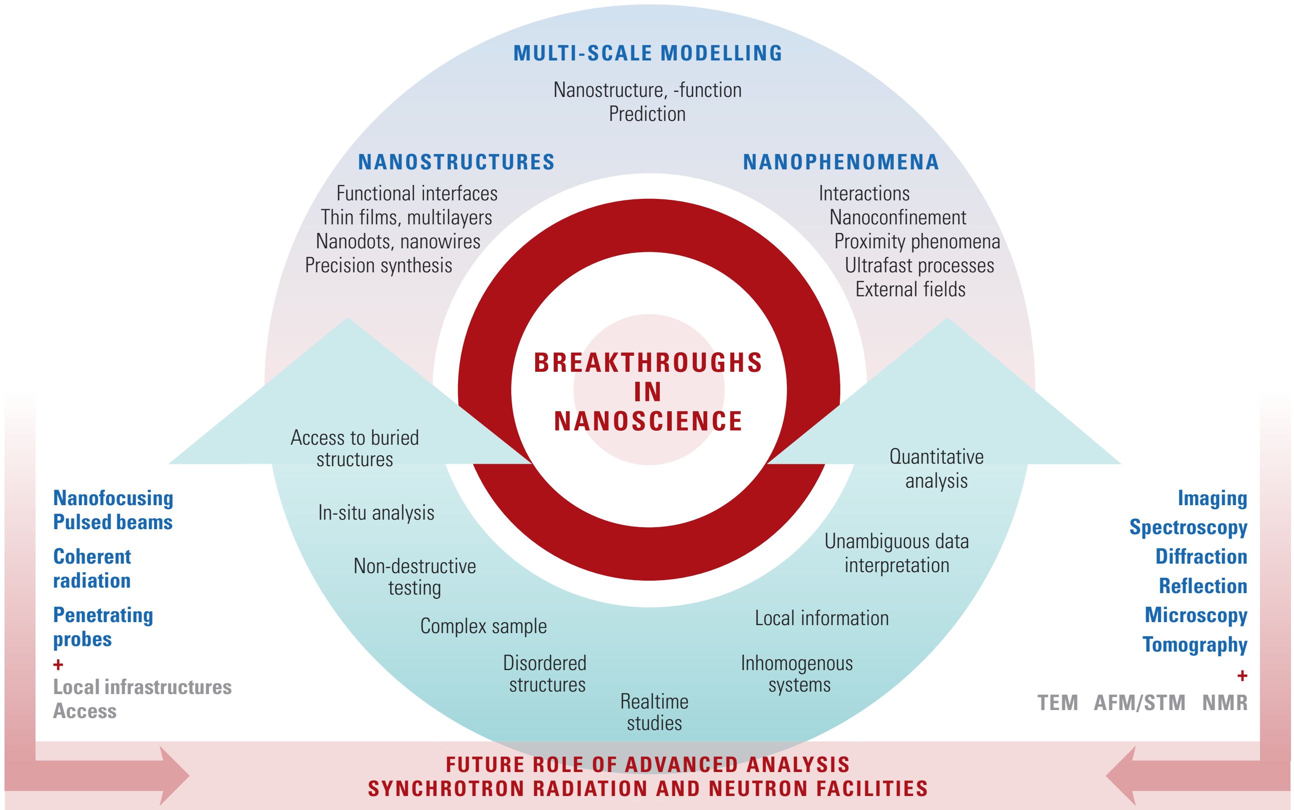


Fig. 11.2.1: Breakthrough areas in nanoscience and the role of synchrotron radiation and neutron facilities.

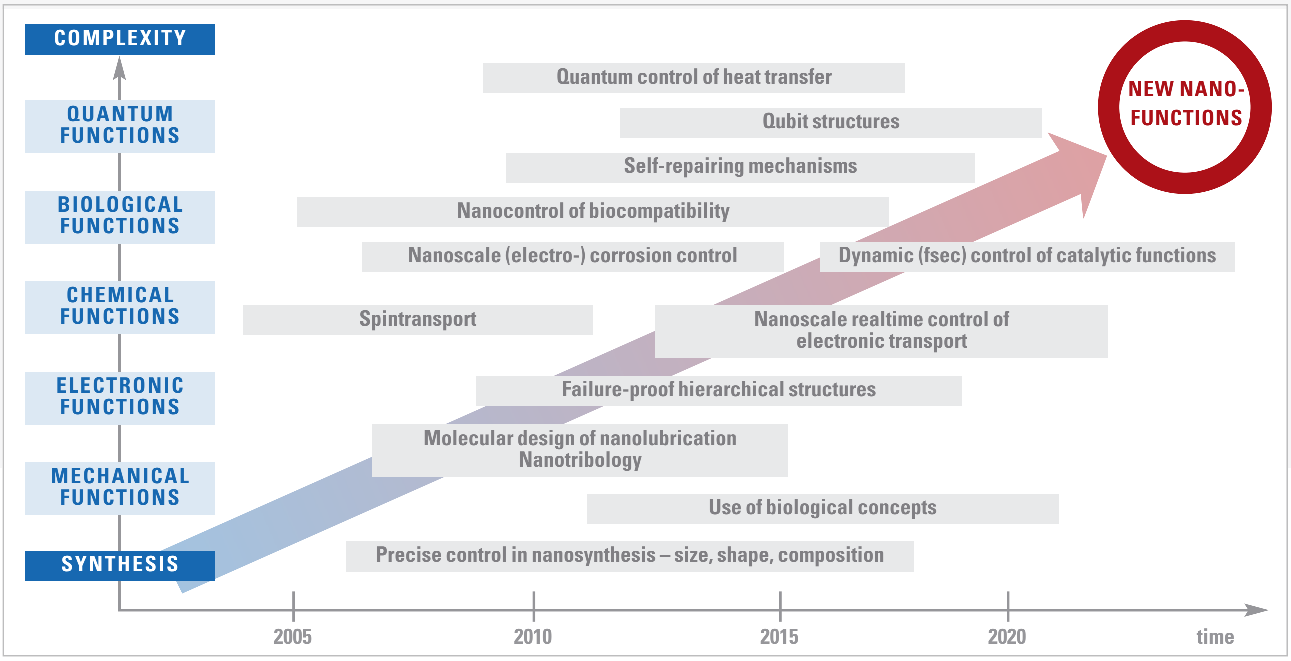


Fig. 11.2.2: Roadmap: Fundamental research in nanoscience.

and -tubes, functionalised surfaces and nanomechanical devices. A further challenge is the atom-controlled design of functional coatings as well as the design of complex hybrid nanoparticles and nanomaterials for:

- Electronics/printable electronics;
- Nanophotonics;
- Nanobiology and biosecurity;
- Nanomedicine.

The synthesis and processing of "intelligent" or "smart" nanoparticles with multiple functions ("3rd generation nanomaterials", see Fig. 11.2.3) requires:

- Combinations of physical-, chemical- and biological synthesis techniques;
- In-situ characterisation under various environments (water, different gases, high pressure);
- Continuous control of particle growth during all individual processing steps;
- Modelling of the synthesis of complex hybrid nanoparticles in order to obtain a microscopic understanding of the growth processes (as interaction between particles).

The unique potential of synchrotron radiation and neutron technologies to study in-situ the growth processes on different length and time scales must be exploited in order to enable a comprehensive microscopic picture/control of the relevant processes. Success in this field will have a strong impact in almost all key technologies, thus a GENNESYS Centre for the precision synthesis of so-called 3rd generation nanomaterials is suggested. The 3rd generation nanomaterials are outside the capacity and expertise of the individual material laboratories and demand for a European approach in which the impact of synchrotron radiation and neutrons is of vital importance.

- **Improved understanding of deformation, fracture and friction at the nanoscale**
  In order to describe deformation and fracture of nanostructured materials as well friction and lubrication in nanomechanical devices, conventional concepts for plasticity and fracture cannot be applied. Synchrotron radiation and neutron techniques play an important and complementary role to tunnelling microscopy, nanoindentation and transmission electron microscopy for observing in-situ and in a non-destructive manner the evolution of defects, such as dislocations, stacking faults and others, during mechanical loading of nanostructures. These experiments should be linked to multi-scale modelling. The ultimate goal is to achieve a detailed atomistic understanding of the underlying deformation, friction and fracture mechanisms including dissipative channels via chemical reactions.

- **In-situ control of structure of solid-liquid and solid-gas interfaces**
  A detailed knowledge of the structure of solid-liquid and solid-gaseous interface at the nanoscale is important for many advanced applications such as catalysis, energy conversion or storage using new nanotechnological approaches. Here, nanofluidics and nanomechanics are playing an important role for controlling the physico-chemical processes.

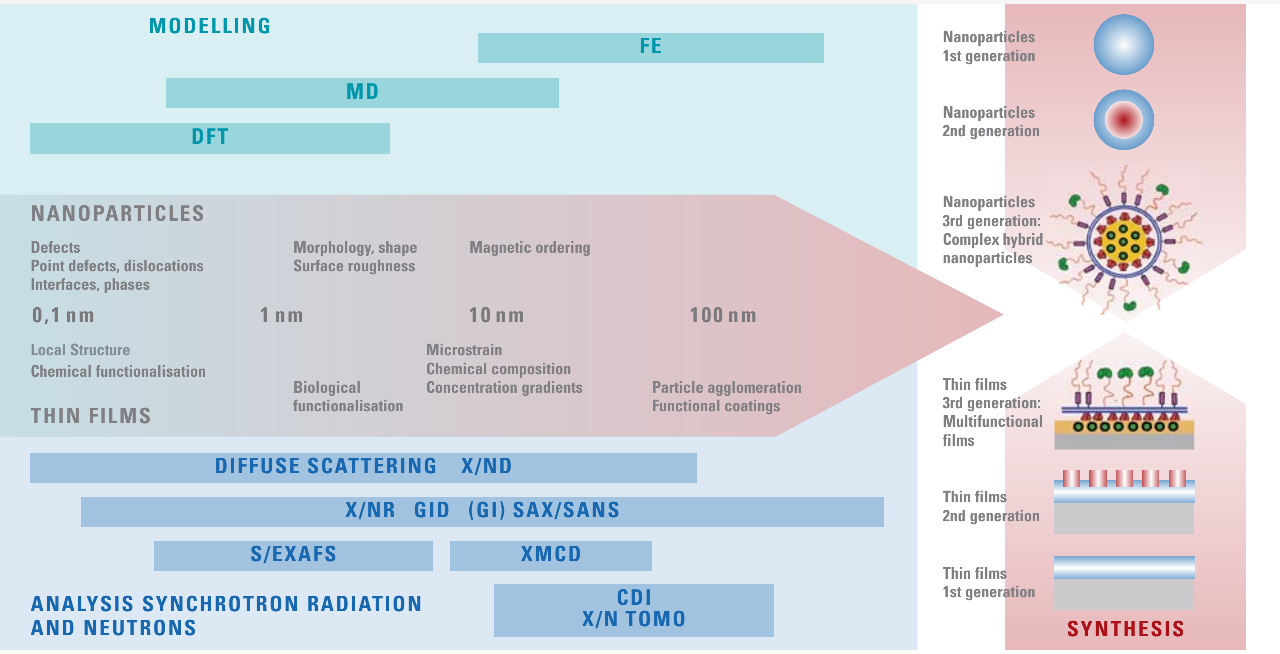


Fig. 11.2.3: Roadmap: nanoparticle and thin film design.

Synchrotron radiation and neutron techniques allow studies in-situ for a more educated approach by providing a detailed microscopic view on the local order/disorder at solid-liquid interfaces which strongly affects wetting and de-wetting processes or the change of surface structures in gaseous atmospheres. As a result, a broader knowledge base is obtained finally enabling the design of functional nanomaterials which are based on the knowledge of underlying reactions and mechanisms.

- **Behaviour of nanomaterials in extreme environments**
  Future applications of nanomaterials will include extreme environments, (i) extreme temperatures and pressures (as in transport and space exploration or in fusion reactors), (ii) harsh chemical conditions (as in corrosive atmospheres), (iii) high electric and magnetic fields (as in fusion reactors) and (iv) extreme mechanical loads (as in transport and space technologies). The challenges are, on the one hand, to harden nanomaterials making them resistant against such environmental influences, on the other hand, exploit such extreme conditions for the discovery of new materials with entirely unique properties, see Fig.11.2.4 (i.e. synthetic high pressure chemistry for the creation of a new generation catalysts).

The roadmaps of synchrotron radiation and neutron centres must be supported sufficiently to enable an internationally leading technology.

- **Functional interfaces in a reactive environment: nano-oxidation and nanocorrosion** (Fig.11.2.5)
  Oxidation and corrosion of highly reactive nanomaterials (alloys, oxides) determines the stability, functionality and long term performance in their working environment. The control of oxidation and corrosion under operational conditions is of utmost importance for the enhanced performance of catalysts involved in industrial applications ranging from fuel cells and chemical production to electronic sensors for automotive and environmental monitoring applications, magnetic storage media or optical coatings. As corrosive media act oxygen, nitrogen, SO_2 or other gases or plasmas; water, or acids under electrochemical control.

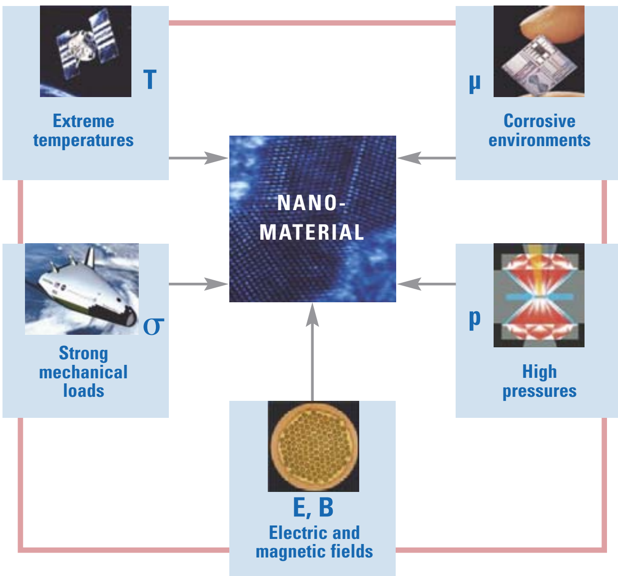


Fig. 11.2.4: Nanomaterials testing under extreme conditions.

Using synchrotron radiation and neutrons as an in-situ probe, corrosion processes can be monitored on the atomic scale in-situ, in real-time down to picoseconds under realistic, industrial conditions as a function of the corrosion potential and at high temperatures. Only these in-situ studies will give the necessary atomistic insight to tailor and improve nanomaterial corrosion properties, avoiding trial and error procedures. They will provide the input for a data base on nanomaterial oxidation/corrosion and protective materials for industrial applications.

The knowledge, prediction and control, how nanomaterials behave and eventually deteriorate under corrosive conditions, will bring increased security to a European society becoming increasingly more dependent on nanotechnological systems and structures.

- **Development of bio-nanofunctions**
  To investigate the synthesis and the assembly of new functional nano-materials based on nature (where such processes have been refined over millions of years) are of utmost importance. Understanding the complex relations between nano-scale structure and function in biological materials will provide invaluable insights into the "tricks of the trade" and perhaps save years of development, in addition to enabling advances in nanomedicine, bio- and biomimetic materials. There has been noticeable progress in the development of novel bio-mimetic material structures. In the future smart designs, there is the challenge to get to grips with nature's approach to the dynamical control of processes. This will lead to a myriad of new applications including biosensors, micro-fluidic devices and smart scaffolds for tissue engineering.

Key to progress is the molecular insight into the structure and function of the bio- and bioinspired nano-units which requires advanced analytical tools including synchrotron radiation and neutrons.

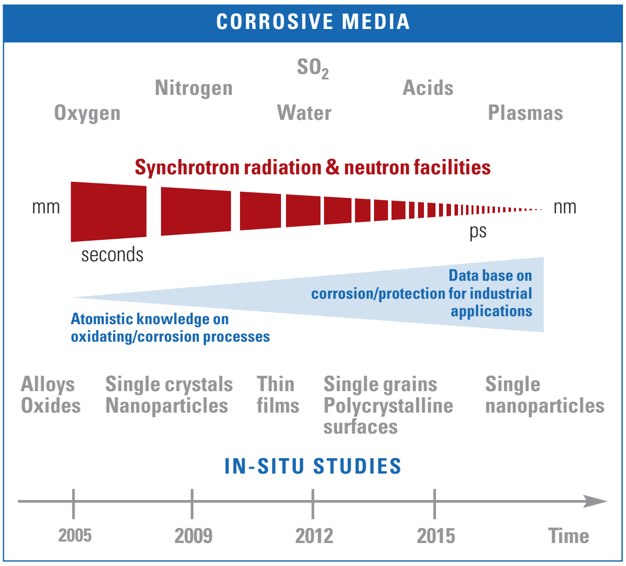


Fig. 11.2.5: Future research for nano-oxidation and corrosion.

- **Detection of single impurities in nanomaterials**
  Future generations of nanotechnologies, from quantum computation to light harvesting for energy, will be based on new nanoscale materials and devices that operate with only a few electrons. In the ultimate case one – and only one – atom must be introduced into a host nanosystem to realise the intended function. Potential synthesis routes should be developed to achieve single atom control; they cannot be successful in the absence of the capability to detect and visualise a single atom buried inside an object. Quantum computers and ultra dense magnetic storage will be based on nanoscale devices whose behaviour is dependent on the position and interactions of one single atom placed within the host nano-architecture.

Synthetic and analytical (in-situ) technologies must be developed to control single impurities in functional nanoarchitectures. For such analytical capabilities, the development of x-ray nanobeams with sufficient intensity is mandatory. Possible new detection schemes are x-ray fluorescence nanotomography, x-ray photoemission using nanobeams and STM detectors.

- **Standardised databases – computer models – experiments at the fingertips**
  The creation of a European data bank should be encouraged; it would promote cooperation in data analysis, the interchange of information between experimenters and facilitate data modelling. Academic and industrial research must, over the next decade, enable individual researchers to exploit standardised and evaluated databases which would reside on several nodes of the universal computing grid, as well as on more local resources ranging from a personal computer to an industry lab or commercial computing centre allowing users to have the full contents of the "data base" at their fingertips whether collecting data at a facility or working from their home institutions.

- **Analytical access to ultrashort timescales**
  The relevant timescale for the dynamics of atoms and electrons in materials under relevant temperatures is in the subpicosecond regime. The ultimate atom – and electron – control of materials thus requires that analytical technologies can master these ultrashort timescales. There are essentially three analytical challenges:
  - Pump-probe analysis of the response of materials and structures;
  - Real-time movies of reactions and atomic and electronic processes;
  - Ultrashort snapshot of liquid functional materials.

  These analytical capabilities are not available today. However, the novel free electron laser (FEL) facilities which are now emerging in Europe carry this ultimate potential to interrogate materials on these timescales.

  The materials science laboratories must establish contact with the FEL facility managers to devise novel instrumentation dedicated to the needs of nanomaterials design.

11.3. KEY CHALLENGES FOR NANOMATERIALS DESIGN

In many areas of science and technology, existing materials have reached a high level of maturity and the rate of development of the technologies which exploit them has decreased. In many such cases, the new found capability to manipulate materials at the nanoscale can offer step changes which regenerate the development cycle.

Neutron and synchrotron sources can help deliver both growth stages of this paradigm, transforming the world in which we live. Information about quantum magnetisation tunnelling in clusters can be obtained by inelastic neutron scattering, leading to completely new devices, while information provided by x-ray diffraction can help to optimise the crystal structure of smart structural materials to engineer the transformation to occur at the required temperature or mechanical stimulus (see Fig. 11.3.1).

New materials, engineered at the nanoscale, are poised to radically transform key technologies in various areas of great social concern, from energy (including fuel cells, sustainable energy generation and transport) to global security (e.g. people and baggage scanning) to healthcare (e.g. microsensors).

The development of nanomaterials and the devices which exploit them require effective integrated relationships, from the physics, chemistry or biology of the local scale through to engineering functioning devices/structures. This cannot be achieved without a new pattern of working which connects theorists and experimentalists more closely with the large-scale facilities, enabling the neutron or synchrotron beam to shed light onto the manufacturing/nano-assembly process or the operation of the device under service conditions (see Fig. 11.3.2).

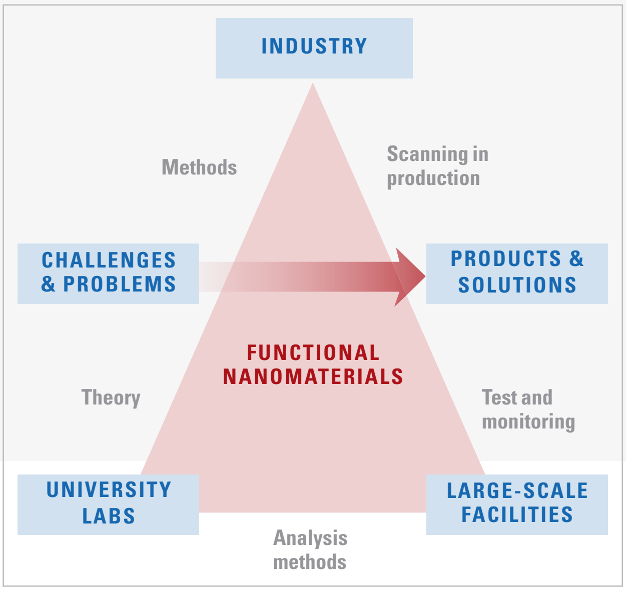


Fig. 11.3.2: Interdisciplinary challenges in the development of nanomaterials.

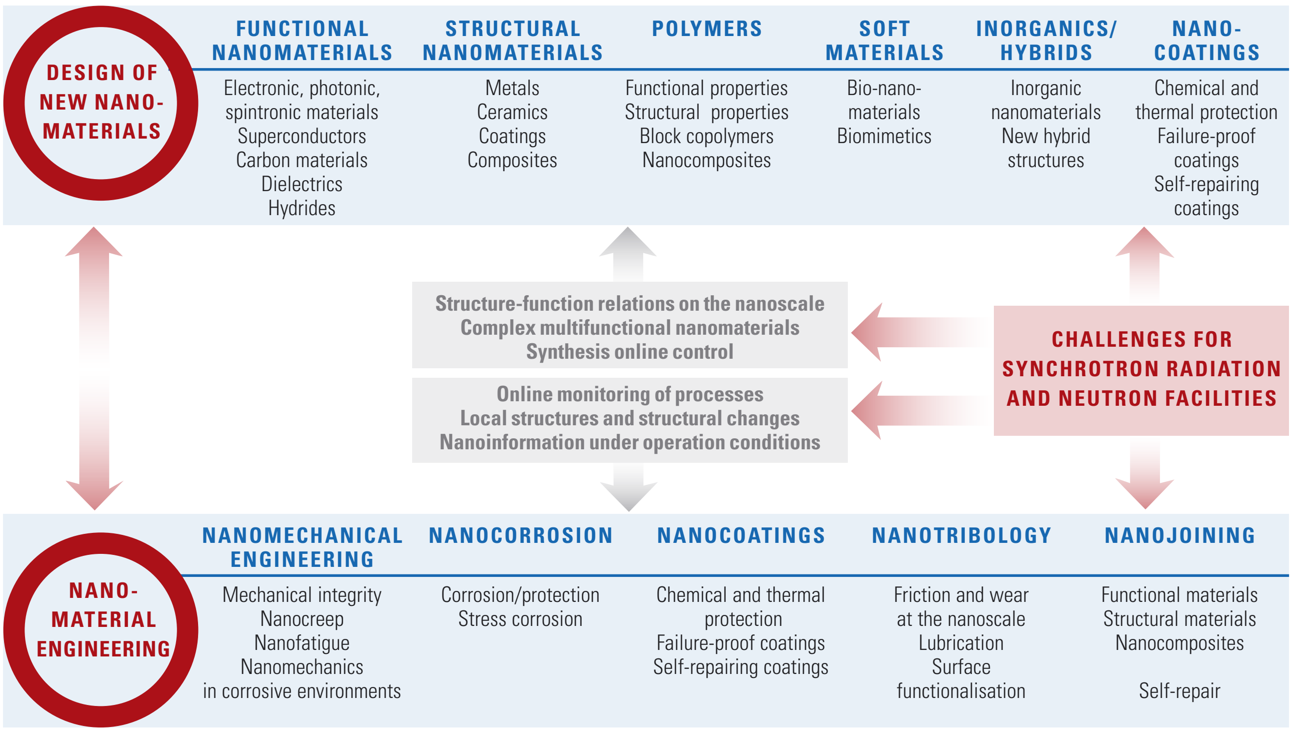


Fig. 11.3.1: Overview of nanomaterials: design and engineering.

11.3.1. NANOMATERIALS FOR ELECTRONICS (see Table 11.3.1)

Although in the next few years, the emphasis of the Si micro(nano) electronic roadmap lies in technological development, solutions will be needed for the mid-term problems facing the era beyond Si-CMOS technology. New and interesting concepts are already taking shape, e.g. the use of single-atomic layers of carbon, graphene, with a whole range of unexpected and very interesting properties.

Synchrotron radiation and neutron facilities will play a key role in the full 3-D characterisation of nanostructures. The main goal is the non-destructive investigation, e.g. chemical and strain analysis, defect characterisation and interface properties with atomic resolution, as well as nanostructure fabrication with atomic control.

11.3.2. NANOMATERIALS FOR PHOTONICS (see Table 11.3.2)

Since the down-scaling of electrical interconnects does not improve their performance, they will be the limiting factor in device miniaturisation. One solution is to replace them with optical connects. Nanophotonic concepts may affect telecommunications, display technology, optical data storage, logic circuits. Tera-Hertz photon sources and detectors will impact security applications, e.g. for real-time screening at airports and other safety checkpoints.

The use of synchrotron radiation and neutrons is an essential tool in the fabrication (lithography) and material characterisation technology, the detection technology, and the realisation of novel quantum devices.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Develop more powerful chips by continued miniaturisation	Transistor speed by local strains	Optimise fabrication process for strain control	Local strain analysis
	Ultrathin dielectrics: interface properties and porosity	New high κ materials	Combinatorial screening of promising materials
	Transistor optimisation	SOI, metal gate, high-mobility materials (e.g. III-V) on Si	High resolution in-situ characterisation
	3-D control of doping profiles	Optimise fabrication process	3-D information with atomic resolution
	Interconnect strains	Low κ insulator, temperature profile of fabrication process	Full structural control during process
	CVD: introduction of hydrogen, pores, voids	Process optimisation	In-situ detection of hydrogen
	Beyond 22 nm technology: End of the Si-CMOS ?	Nanowires, nanotubes, molecular electronics Graphene sheets Exploratory basic research	High resolution analysis of new architectures at all length scales

Table 11.3.1: Key challenges in electronic nanomaterials.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Replace electric interconnects by optical ones	Fabrication of photonic crystals	Lithography	Characterisation
	Nanowires as photon emitters or detectors	Self-assembly	X-ray lithography
	Single photon sources and detectors	Self-assembled growth on pre-patterned substrates	Materials characterisation
	("Photons on demand")	Addressable quantum dots	Materials characterisation
Quantum communication	Entangled photon sources	Quantum dots	Materials characterisation

Table 11.3.2: Key challenges in photonic nanomaterials.

11.3.3. MAGNETIC NANOMATERIALS (see Table 11.3.3)

Research in nanomagnetism is primarily motivated by applications such as spintronics, magnetic sensing and ultra-high-density magnetic recording, with targeted storage capacities larger than 1TB/inch^2. During the past decade, nanoscale magnetic devices for data storage have had a revolutionary impact on computers and information technology. In the context of the emergence of spintronics, the discoveries of spin-injection, giant-magnetoresistance and tunnelling magnetoresistance created an interest in applying in addition to their electronic properties also the spin degrees of freedom of electrons. All these properties vary dramatically when entering the nanoscale.

11.3.4. SUPERCONDUCTING NANOMATERIALS

(see Table 11.3.4)

Layered superconducting nanomaterials are starting to find applications in technologies. A key barrier is the control of stoichiometry, interfaces, patterning, and self-assembly. Thus, characterisation methods with sufficient sensitivity have to be developed, as well as theoretical and computational methods which will allow achieving a better understanding of electron, spin and fluxon confinement phenomena. This requires detailed high-resolution characterisation of the microstructure of the devices and a correlation between structure, properties and fabrication parameters.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Non-volatile magnetic memory	Switching of states longevity (energy barriers between states)	Understand mechanisms of switching, determine and engineer energy barriers	Magnetic scattering, time-resolved studies, spectroscopy of energy levels
	Fabrication of patterned arrays	Lithography	X-ray lithography
Spin-based devices	Domain wall propagation in magnetic material (new memory concept)	Dynamics of domain walls (fundamental science)	Magnetic scattering with local and time resolution. Pulsed polarised neutrons
	Spin transistor: spin dynamics, ferroelectric gate and SET coupling	Investigation of spin dynamics (precession)	Magnetic scattering with local resolution
Control of magnetisation in nanostructured magnets	Change of magnon spectra as a function of size	Determination of magnon band structure	Inelastic scattering (extremely challenging due to very small scattering volumes)
	Change of magnetisation with shape, size	Determination of size effects Determination of exchange bias	XMCD, polarised neutron scattering
	Interaction in arrays Change of magnetisation due to external stimuli	Magnetisation under applied fields, pressure, chemicals	Time-resolved XMCD and magnetic scattering

Table 11.3.3: Key challenges in magnetic nanomaterials.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Search for new superconductors	New synthesis and doping techniques	Synthesis at extreme conditions Combinatorial search	Combinatorial in-situ characterisation of material properties
Control of superconducting heterostructures	Proximity effects	Controlled deposition Optimisation of interface microstructure	In situ determination of surface and interface properties
Engineering of artificial superlattices	Fine tuning of interface properties	Better control of deposition parameters	Nondestructive in-situ monitoring of emerging structures during deposition
Control of Josephson devices & sensors	Reproducibility Charge, spin and energy transfer	Nanoscale control of interfaces Quantum measurements	Characterisation of interface structures
Improving bulk sample single crystal purity	Control of defects, dopants and disorder	New methods of temperature gradient and nucleation control	In-situ control of crystal growth

Table 11.3.4: Key challenges in superconducting nanomaterials.

11.3.5. MECHANICAL PERFORMANCE OF FUNCTIONAL NANOMATERIALS (see Table 11.3.5)

Better structural performance of nanomaterials will guarantee mechanical stability of nanodevices and thus will impact the development of all key technologies. Fundamental studies of the mechanical behaviour of nanostructures include the microscopic understanding of the:

- Three-dimensional mechanical response of nanostructures to external strain ("diagonal mechanical response functions");
- Mechanical response of nanostructures to electronic, magnetic and thermal stimulation ("off-diagonal mechanical response functions") and vice versa (important for the development of smart materials);
- Effect of substrate interactions

11.3.6. SMART STRUCTURAL NANOMATERIALS (see Table 11.3.6)

A whole raft of smart materials with properties engineered on the nanoscale is emerging:

- Piezoelectric materials are materials that produce a voltage when stress is applied. Since this effect also applies in the reverse manner, a voltage across the sample will produce stress within the sample. Suitably designed structures made from these materials can therefore be made that bend, expand or contract when a voltage is applied.
- Shape memory alloys and shape memory polymers are thermo responsive or mechanically responsive materials where deformation can be induced and recovered through temperature changes. Magnetic shape memory alloys are materials that change their shape in response to a significant change in the magnetic field.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Improved performance of electronic microdevices	Dislocations, defects, strain can hamper performance	Better understanding of defects and their effects	Combination of inelastic studies and probing of structure/strain by diffraction.
Magnetic devices	Poor understanding of mechanical-magnetic interactions	Better understanding of defects and strain on magnetic nanodomains	Combination of muon studies and probing of structure/strain by diffraction.

Table 11.3.5: Key challenges for mechanical interactions of functional nanomaterials.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Piezoelectric actuators	Low levels of actuation	Better understanding of structure/ piezo electric behavior (e.g. near the morphotropic phase boundary in PZT)	High energy synchrotron radiation diffraction can probe the structural transition and microstresses in-situ under applied electric fields
	Low forces		
	Tunability of transformation to useful thermal or mechanical domains		
Shape memory alloys	Low levels of actuation	Mapping of the structure/ transformation relationships	In-situ neutron or synchrotron experiments under conditions of changing temperature or applied load
	Low mechanical		
	Tunability of transformation to useful thermal or mechanical domains		

Table 11.3.6: Key challenges for smart materials.

11.3.7. MICROELECTRONIC MACHINES

(see Table 11.3.7 and Fig. 11.3.3)

MEMS bring together silicon-based microelectronics with micromachining technology, making possible the realisation of complete systems-on-a-chip promising to revolutionise nearly every product category. MEMS is an enabling technology allowing the development of smart products, complementing the computational ability of microelectronics with the perception and control capabilities of microsensors and microactuators.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
To develop machines capable of many actuations	Degradation of electromechanical performance	Means of characterising electromechanical performance	In-situ diffraction and imaging experiments using micro-beams as a function of extent of life
	Poor fatigue performance	Methods for studying structural degradation under fatigue	
Tailoring performance	More capable smart materials	Better understanding of structural transitions and their triggers	Phase mapping under electrical, magnetic and externally applied loads by neutron or synchrotron diffraction
Manufacturability issues	Interfacing and packaging issues	Better understanding of machine-package constraint effects	Studies of strain at the microscale

Table 11.3.7: Key challenges for microelectronic machines.

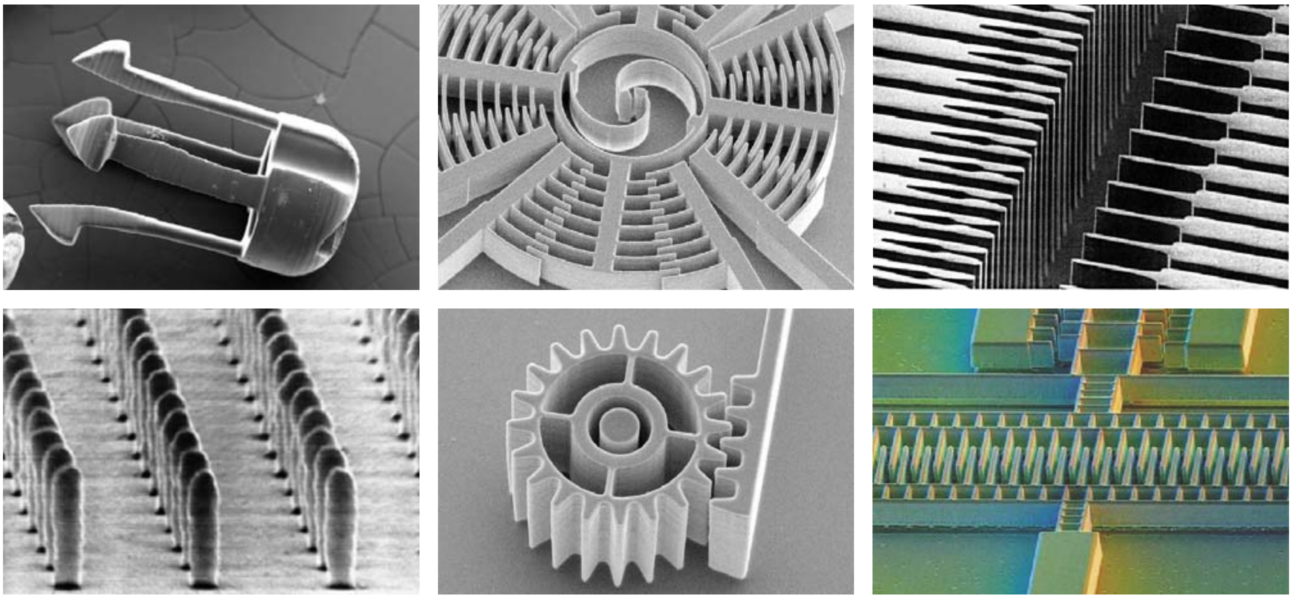


Fig. 11.3.3: Examples of micromachines.

11.3.8. NANOSTRUCTURED METALLIC MATERIALS

(see Table 11.3.8)
Improved understanding of solidification, recrystallisation and phase equilibria could be used to develop a whole new range of nanostructured metals, intermetallics and nanocomposites.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Bulk metallics with tailored nanostructures	Lack of thermodynamic modelling capability for complex many component systems	Means of collecting phase data quickly as a function of temperature to refine/develop thermodynamic data	Fast synchrotron diffraction studies at temperature
	Better understanding of deformation/ recrystallisation relations	Methods for studying recrystallisation kinetics in 3-D	3-D X-ray microscope
	Instability of nanograin-sized metals	Methods for studying grain growth	
To develop tough intermetallics	Large number of possible alloys and treatments	Quick methods of collecting phase data for multicomponent systems	Fast turn around diffraction
	Poor understanding of optimal structures from a toughness viewpoint	Means of characterising damage evolution in nanoceramics	High resolution imaging experiments by synchrotron tomography
To develop new nanocomposites	Effective means of making metallic composites with dispersed nanophases or layers	Means of studying phase morphologies at nanoscale as a function of processing	SAXS/SANS
		Means of characterising damage evolution in nanoceramics	High resolution imaging experiments by synchrotron tomography
Nanomaterial coatings for resistance to temperature, corrosion and biological fluids	Ensuring coating adhesion	Stress determination in nanolayers	Strain measurement in nanocoatings using highly-focussed beams
	Reducing coating stresses	In-situ testing of coating response under in-service conditions	
	Monitoring coating performance in-situ	Extrapolation of local stress in nano-crystallites to macroscopic behaviour	
Materials with higher toughness, better fatigue, creep, corrosion resistance	Understanding the link between nanostructure and bulk mechanical response	Understanding the link between crystallographic texture in nanostructured materials and bulk elastic behaviour	Simultaneous determination of stress and texture
	Engineering of nanostructures for improved mechanical behaviour		
Understanding of the progression of damage mechanics at the nanoscale; Development of 'self-healing' materials and coatings	Conventional fracture mechanics principles do not apply to damage in nanolayers	Characterisation of failure processes through the nanostructure	Identifying the mechanistic drivers for damage development
	Designing with materials whose properties vary with time	Development of new design philosophies	Monitoring of damage development in real time

Table 11.3.8: Key challenges for structural nanometallics.

11.3.9. NANOSTRUCTURED CERAMICS (see Table 11.3.9)
The key issue restricting the wide spread use of engineering ceramics is that of toughness; in principle nanoceramics can provide a solution (see Fig.11.3.4). However, turning a nanopowder into a structural ceramic with a nanograin size is a major challenge. The applications of nanoceramics are summarised in Table 11.3.10.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
To develop tough ceramics	Retaining nanostructure of powder in bulk consolidated ceramics.	Means of studying grain size during hot sintering	In-situ size broadening analysis during high temperature sintering
	Poor fatigue performance	Means of characterising damage evolution in nanoceramics	High resolution imaging experiments by synchrotron tomography
Multifunctional nanoenabled ceramics (dielectrics, piezoelectric, magnetics, etc.)	• Availability of large quantities of nanopowders with reproducible quality • Nanoparticle processing and subsequent treatments (incl. low temperature processing and self assembly techniques) • Interfacial reactions and interdiffusion • Quantitative description of structure-property-relationship • Thermal stability of nanoscaled ingredients and structures	• Industrial fabrication of a large variety of nanopowder compositions • New and well-controllable processing technique • Characterisation and modeling of nano-structure-property relationship down to the atomic level • Precise point (atomic) defect control/ engineering incl. dopants	Characterisation of structure at all length scales, high resolution phase analytics, spectroscopy Direct observation of defect chemistry related effects, local high resolution imaging, spectroscopy for identification of point defect type and concentration
Multicomponent nanocomposites	• Matching of chemical and physical properties • Interfacial stability	• Adapted interfacial layers and its processing • Stability esp. at higher temperatures	Characterisation of interfaces, phase formation incl. in-situ investigations
Ceramic nanocoatings (e.g. catalytic, optical, conducting)	• Controlled processing of nanostructures at surfaces and interfaces • Very low temperature processing (e.g. thin film) • Suitable electric performance • Stability and durability of nanostructure and related properties	• Understanding of generation and formation of nanoassemblies from colloidal solutions (incl. self assembly) • Stabilisation of nanostructures esp. at higher temperatures	In-situ observation of phase and particle formation Characterisation of interfaces incl. incorporation of dopants and competing impurities Local stress and property characterisation
Nanoceramic processing (e.g. at lower temperatures)	• Availability of large quantity nanopowders with reproducible properties • Processing of nanopowders with respect to complete technology chain	• Control of interparticle interaction in processing media • Control of grain growth and phase formation	In-situ characterisation of structure and phase formation, spectroscopy

Table 11.3.9: Key challenges for nanostructured ceramics.

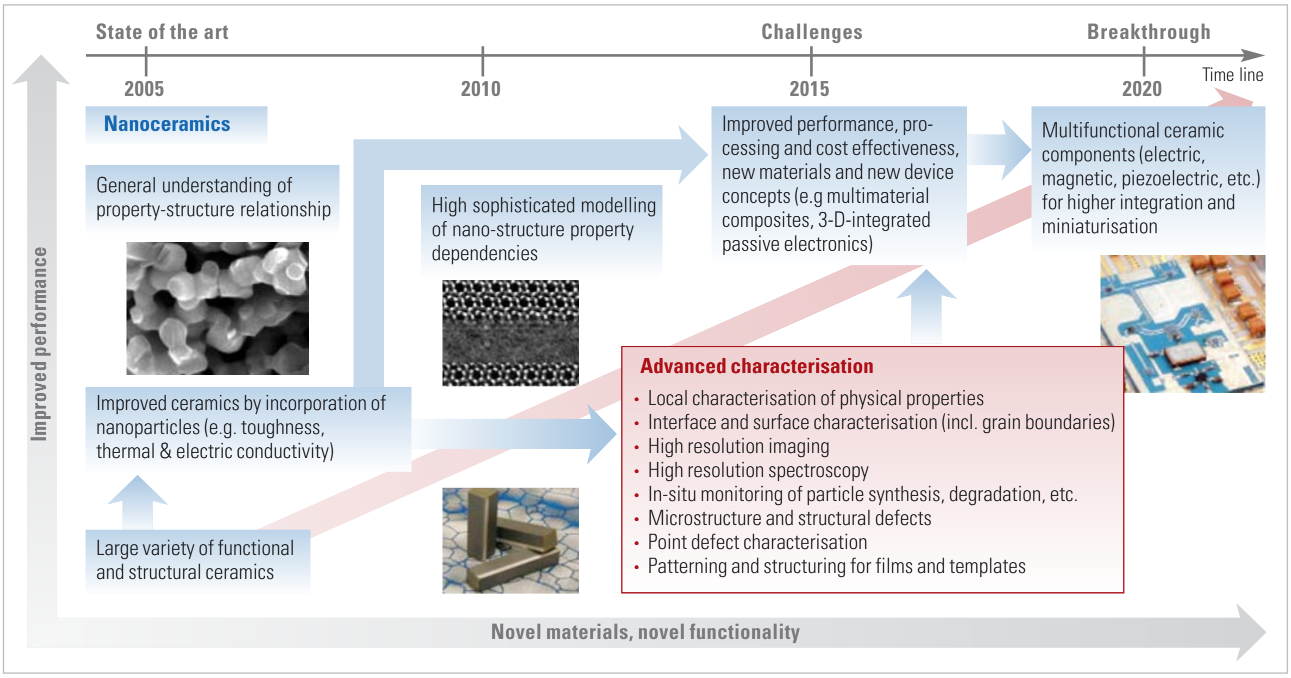


Fig. 11.3.4: Roadmap for nanoceramics.

		R&D KEY ASPECTS	
FIELDS	**APPLICATION**	**FUNCTIONAL CERAMIC PROPERTIES**	**STRUCTURAL CERAMIC PROPERTIES**
Electronics, information & communication	Advanced electronics	Tunability, printable, low-cost, high-temperature, miniaturised, etc.	
	Adaptronic & mechatronic	Functional composites and surfaces	
	Ceramic MEMS integration	"Functional components, bonding & sealing"	
	LTCC boards and modules	"Magnetics, dielectrics, etc., low temp. processing, thermal management"	Thermo-mechanical behaviour
	Ceramic packaging, SiP(system in package)	„Low temp. processing, bonding, sealing"	Thermo-mechanical behaviour
	High density data storage	High-k dielectrics, optics, bistable materials	
	Thermoelectrics	Electric & thermal conductivity	Thermo-mechanical behaviour
	RF-devices	Dielectrics, meta-materials	
	Optoelectronics	Phosphors, optical films & composites	
Energy & environment	High temperature insulation		"Ultra-low thermal conductivity, thermo-mechanics"
	Gas turbine hot parts		Thermo-mechanics, life-time & reliability
	Fuel cell	Ionic & electric conductivity, sealing & processing	
	Combustion	Catalytic surfaces	
	Gas separation membrane	Ionic conductivity	Thermo-mechanical behaviour
	Exhaust treatment	Catalytic surfaces	
	Functional coatings	Anti-adhesion, self-cleaning, etc.	
	Photovoltaic	Optical & electronic behaviour, boards	
	Solarthermic	Optical & thermal behaviour, processing	Thermo-mechanics, life-time & reliability
	Battery	Electro-chemical behaviour, power density	
	Energy storage	Hydrogen storage	
	Air & water purification	Catalytic & bio-active membranes	
Transport & mobility	Sensors & actuators & adapatronics	Piezoelectrics, LTCC-boards, SiP, etc.	
	Drives	Piezoelectrics	
	MEMS	"Functional components, bonding & sealing"	
	Combustion engines	Functional coatings	
	Auxiliary power units, alternative engines	Fuel cells (SOFC)	
	Energy harvesting	Piezoelectrics, thermoelectrics	
	Battery	Electro-chemical behaviour, power density	
	Exhaust treatment	Catalytic surfaces	
	Brake system		Fiber composites
Industrial equipment	Bearings		Surface quality, precision processing, lubrication
	Forming & cutting tools		Mechanical performance, life time, thermal stability
	Tribo-coatings		Wear resistance, lubrication
	Super-hard components		Hardness, toughness
	Metal-ceramic joining	"Ceramic" solders	Thermo-mechanical behaviour
Health	Bone & tissue substitutes	Bio-compatibility	Mechanics, corrosion
	Tooth substitutes	Esthetics	Mechanics, precision processing
	Implants	Bio-compatibility, bionic	
	Intelligent implants	Bio-electric behaviour (interface)	
	Imaging & contrast agents	Carrier particles	
	Tumor therapy	Magnetic, electromagnetic absorption (carrier particles)	
	Drug delivery	Carrier particles	
	Bio-sensors	Thin films (piezoelectric, optical, etc.)	

Table 11.3.10: Application potential for nano-scaled structural and functional ceramics.

11.3.10. NANOSTRUCTURED POLYMERS AND BIOMATERIALS

(see Table 11.3.11)

Future priority research areas for the development of polymer nanomaterials are shown below.

POLYMERS	BIOPOLYMERS
· Designer supra-molecular assemblies · Conducting polymers · Organic magnetic materials · Micro- and nanofluidics · Quantum materials · Smart stimuli responsive macromolecules · Structure-property relationships in processings · Super-critical fluid complexes · Interfaces of complex materials · Adhesion and lubrication (molecular and macroscopic)	· Targeted drug delivery vehicles · Genomics · Multiprotein complexes · Structure based drug design · Membrane proteins · Bioadhesion and biocompatibility · Biosensors and detection devices · Biomimetic polymers and materials

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
To develop polymer/ quantum-dot systems with unique optical and electronic properties	Processing to obtain dispersed nanocomposites free of nanoparticle aggregation	Quantum-dots tailored with electronically active polymers	Characterisation of nanoparticles in bulk, surface layer, multilayer and micellar type matrices
		Exploration of nanoparticle/matrix interphase	SAXS and SANS (contrast variation)
Exploiting morphological nanoscale effects for improved polymer properties across a wide range of temperature and mechanical conditions	Thermal stability for higher temperature applications	Understanding of chain micro-structure/nanoscale/properties relations	Determination of local and large-scale structures within polymers on thermal treatment
	Optimal mechanical performance	Dynamic deformation studies	Morphological developments on dynamic mechanical treatment
	Fabricating nanocomposites with high strength and toughness	Characterisation of load transfer between phases	Internal strain measurements
	Experimental: limitations in scattering power	Deuteration facilities for small-scale material prototypes	Contrast variation for resolving nanostructural details
Polymers exploiting biomimetic effects Development of materials with high biocompatibility	Hydrogenated polymers cannot in general be studied using neutrons	Deuteration facilities for small-scale material prototypes	Identification of systems with beneficial mechanisms
	Understanding the structure property relations of biomaterials	Studies on natural materials, nature mimicking materials and their composites	Molecular and superstructural characterisation
Bottom-up fabrication of block copolymer based nanostructures	Tuning molecular parameters and microphase domains	New synthetic pathways (ATRP/NMP/RAFT) Modelling and simulation	Determination of structural order
Create intelligent gels	Fabrication of intelligent stimuli responsive gels involving nanoparticles	Basic knowledge on (bio) polymer and polyelectrolyte nanoparticle interactions	Chain dynamics during gelation/kinetics of gelation/superstructure in gels
Cost-effective nanocomposites	Achieving a high quality of the dispersed phase	Means of studying phase morphologies, ideally during processing	In-situ SAXS/WAXS/SANS

Table 11.3.11: Key challenges for nanostructured polymers.

Neutron- and synchrotron radiation-based analytical techniques are indispensable tools for the further development. Their role is summarised in Fig. 11.3.5.

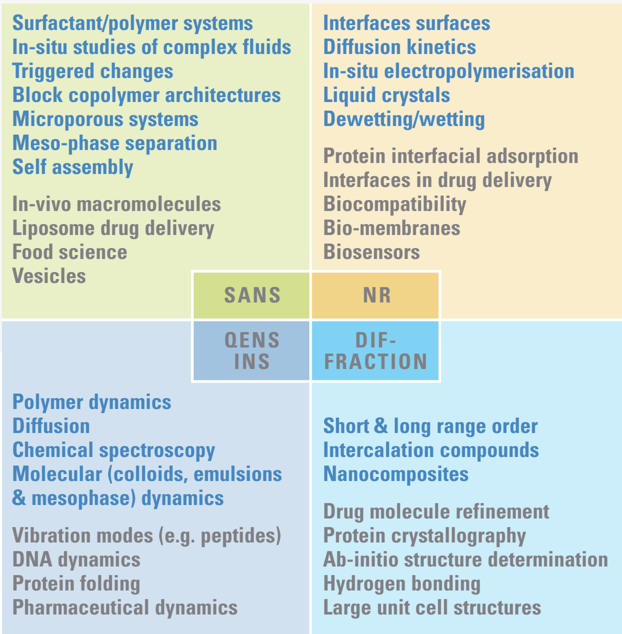


Fig. 11.3.5: Role of synchrotron radiation and neutrons for: yellow (synthetic polymers) and white (biomaterials).

Neutron- and synchrotron radiation-based analytical techniques are indispensable tools for the further development. Their role is summarised in the subsequent diagramme.

The large-scale facilities should provide:
- SAXS, XAFS, IR, imaging, hard-soft x-ray microscopy techniques;
- Surface-sensitive quasi-elastic neutron scattering instruments;
- Routine ultra-small angle neutron scattering capabilities;
- At neutron facilities: full synthesis and deuteration support facilities;
- Complementary characterisation equipments;
- Theory and data analysis support;
- Engineering support for sample environment design and manufacture.

11.3.11. SOFT AND BIOLOGICAL MATTER

Soft matter materials are ubiquitous in every-day life. Motor oil, paints, food stuff, pastes, plastics and rubbery materials, tires, health- and skin-care products, pharmaceuticals, cosmetics and diapers are all examples of soft materials. A common feature of all these materials is that, on the microscopic scale, they are made of macromolecular building blocks with a typical size in the range from nano- to micrometers. The most frequently encountered building blocks are colloids, polymers, and surfactant molecules. Colloids are small, solid

STATE-OF-THE-ART	FUTURE NEEDS & CHALLENGES
• **Single-component systems** - Polymers - Colloids - Surfactants	• **Complex building blocks** - Synthesis - Genetic engineering - Organic-inorganic hybrids - Phase behaviour
• **Self-assembling systems** - Oil-water-surfactants mixtures - Block co-polymers - Telechelic polymers - Colloid-polymer mixtures	• **Composite systems** - Nanocomposites (nanocolloids in polymer matrix) - Polymer mixtures (linear/linear and linear/branched) - Viscosity modifiers - Colloids in viscoelastic solvents - Colloid-surfactant mixtures - Multi-component membranes - Membranes with inclusions
• **Bilayer membranes** - Elasticity - Mechanical deformation - Thermal fluctuations	• **Biological systems** - Blood cells - Active gels - Protein dynamics - Actin networks - DNA complexes - Cell adhesion
• **Colloids** - Gels and glasses - Phase behaviour - Depletion phenomena - Tunable interactions	• **External fields** - Combination of fields (shear flow/electric, shear flow/thermal gradients) - Multi-particle laser tweezer manipulation - Response of composite materials - Manipulation toolbox - Directed assembly - Micro-fluidics - Wetting
• **Polymers** - Various architectures (linear, branched, dendrimers) - Glasses - Reptation dynamics - Rheology	
• **External fields** - Shear flow - Electric fields - Thermal gradients - Laser tweezers	

Table 11.3.12: Research needs in soft matter

particles. The geometry of these colloidal particles varies from spherical to disk- or rod-like. Polymers are very long macromolecules made from a single (or a few) identical units called monomers. The characteristic feature of polymers is that they are very flexible so that entropy determines their properties. Surfactant molecules have an amphiphilic nature, in the sense that they consist of a polar, hydrophilic head and a hydrocarbon, hydrophobic tail. This amphiphilic character implies the tendency for these molecules to self assembly at oil-water interfaces, which drastically reduces the interfacial tension.

The building blocks of biological cells have many properties in common with synthetic soft-matter systems. For example, the plasma membrane of cells is made of amphiphilic bilayers. There are also many bio-polymers, like DNA, F-actin and microtubules. These polymers have a very different flexibility as compared to synthetic polymers, in order to fulfill their different biological functions. A very important class of biological molecules is proteins, which have polymeric, amphiphilic as well as colloidal properties.

The trend in soft-matter research in recent years is towards the study of more complex systems. In the future, the investigation of soft-matter systems with increasing complexity will be the main direction of research (see Fig. 11.3.7 and Table 11.3.12). The complexity of soft materials originates from the following four sources.

- **The complex nature of the building blocks**
  The materials which will be important in the future consist of building blocks, exhibiting properties that do not fall within one of the traditional classes of colloids, polymers and surfactants, but share properties of several of them. Examples are block co-polymers that have a polymeric as well as an amphiphilic character, Janus particles which are both colloids and surfactants, or viruses which can be regarded as protein shells as well as colloidal particles. A schematic overview of the macromolecular "tool box" is shown in Fig. 11.3.6.

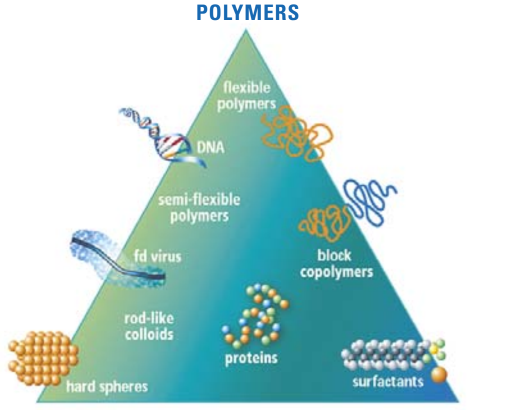


Fig. 11.3.6: The nanofood triangle.

- **Mixtures of various types of soft matter components in a single material**
  New material properties emerge when different types of soft-matter building blocks are mixed. By mixing different components, new materials can be designed with controlled optical, mechanical, rheological and thermal properties, which cannot be achieved using single components. A recent example is nanocomposites, where small colloidal particles are embedded in a polymer matrix, which enhances the mechanical and flow properties of polymer melts.

- **External fields to control material properties**
  Soft materials respond very sensitively to external fields like flow, electric and magnetic fields, thermal gradients and laser fields. This sensitivity arises from the mesoscopic size of the building blocks and the corresponding long relaxation times. External fields are therefore ideally suited to manipulate the microscopic structure and thus the macroscopic properties of soft materials. For example, laser tweezers are becoming a versatile tool to manipulate a large number of colloidal particles simultaneously, in order to create materials with designed microstructural order.

- **Biologically-inspired materials**
  Many biological macromolecules can be used as model systems in soft-matter research. These macromolecules have unique properties which cannot be realised easily with synthetic materials. A very important example is DNA, where the complementarity of the two strands can be employed in many ways to construct highly specific interactions. Genetic techniques can be used to synthesize new types of bio-macromolecules with a very high degree of mono-dispersity. On the other hand, the physical principles of structure formation in synthetic soft materials will help to unravel the mechanisms of processes in living cells. A qualitatively new feature in living systems is the importance of active processes. An example is polymerisation/de-polymerisation of F-actin and microtubules, and active transport due to motor proteins.

Future role of synchrotron radiation and neutrons

The investigation of complex, multi-component soft materials requires detailed knowledge of the structure and dynamics of the individual components. Neutrons are particularly well-suited because of the possibilities of contrast variation. This enables the study of the behavior of all individual components. The commissioning of new spallation sources considerably extends the accessible range of length and time scales, which then covers most of the scales that are relevant in soft matter research (see Fig. 11.3.8).

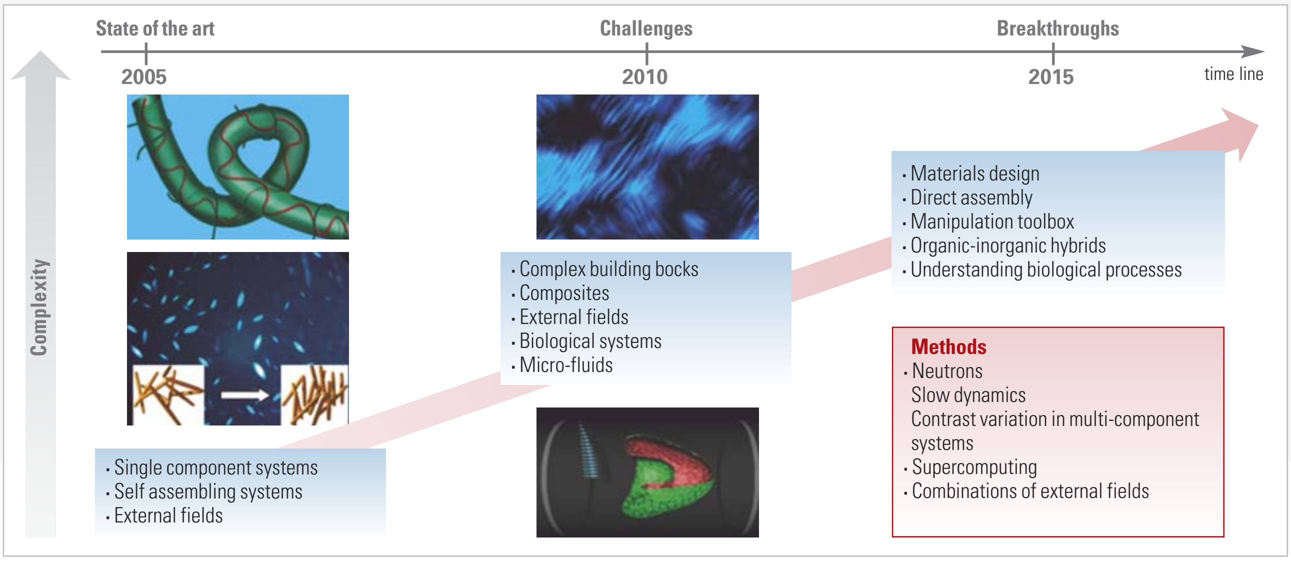


Fig. 11.3.7: Research roadmap for soft and biological matter.

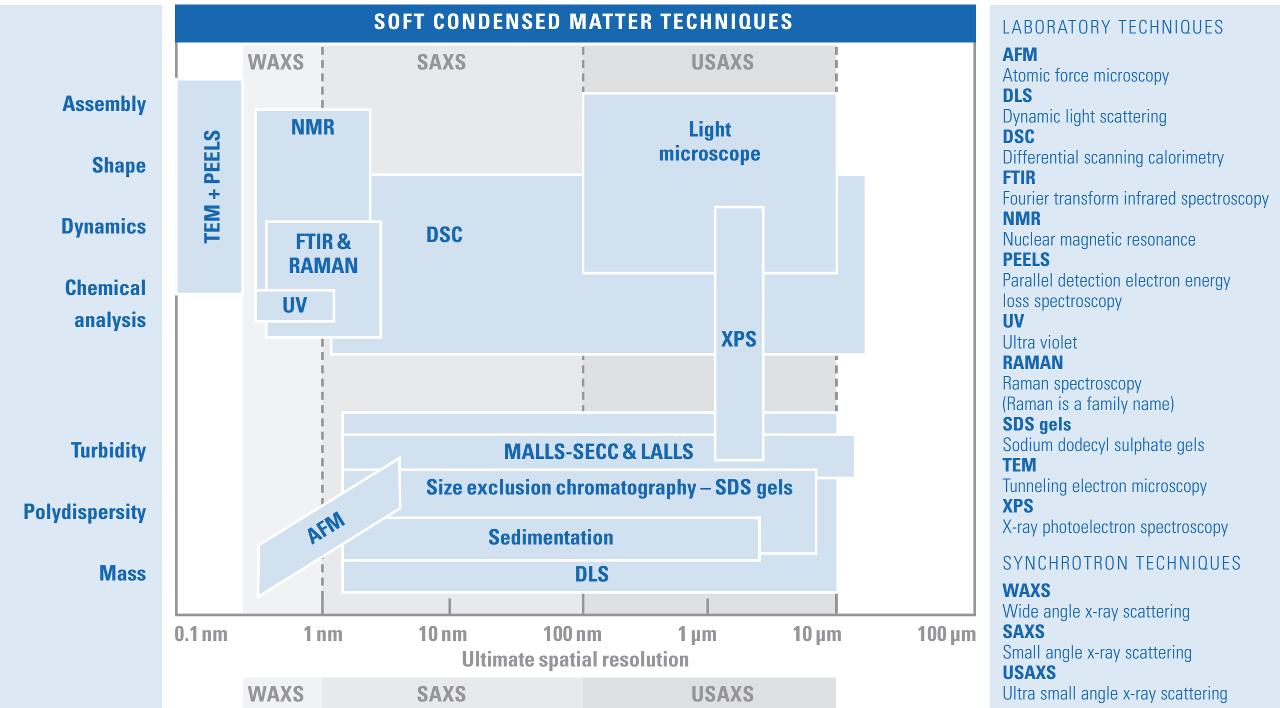


Fig. 11.3.8: Soft condensed matter techniques

11.3.12. MULTI-SCALE STUDY OF COMPOSITE MATERIALS

Nanocomposites:

- Nanotube containing structures
- Nanoclay containing materials
- Nanostructured co-polymers

The ultimate aim is therefore to establish a consistent hierarchical framework of 3-D characterisation tools and 3-D modelling tools that can predict the mechanical properties (strength and fracture toughness) of composites from the basic properties of fibre, matrix and interface, accounting for the presence of defect. Experimentally the requirement is to perform in-situ

- 3-D mapping of the topology of the structure and its evolution, in particular defects and the size, form and roughness of cracks;
- 3-D mapping of the deformation (the elastic and plastic strain fields).

Fig. 11.3.9 illustrates how damage propagation can be characterised as function of scale using large scale facilities in the case of a wind turbine blade. Relevant simulation tools are also indicated.

11.3.13. NANOCOATINGS

Drivers for nanostructured coating systems are as follows below (see Fig. 11.3.10):

- **Smart nanostructured coatings**

To tailor multi-functionally smart coating systems with embedded sensing technologies to provide and to sense variable intrinsic responses to external stimulus: i.e. coatings respond to local chemical activities and develop optimum oxidation or hot corrosion protection; impact and damage tolerance to be engineered using multilayered architectures such that fracture of the ceramic component and plasticity in the metallic components can be minimised, resulting in a near elastic response from the composite surface. The development of anti-erosion coatings could offer great potentials for multiple technologies.

- **Self-diagnostic coatings**

To develop new self-diagnostic multi-functional nano-coatings These differ from "smart structures" by providing some active stimu-

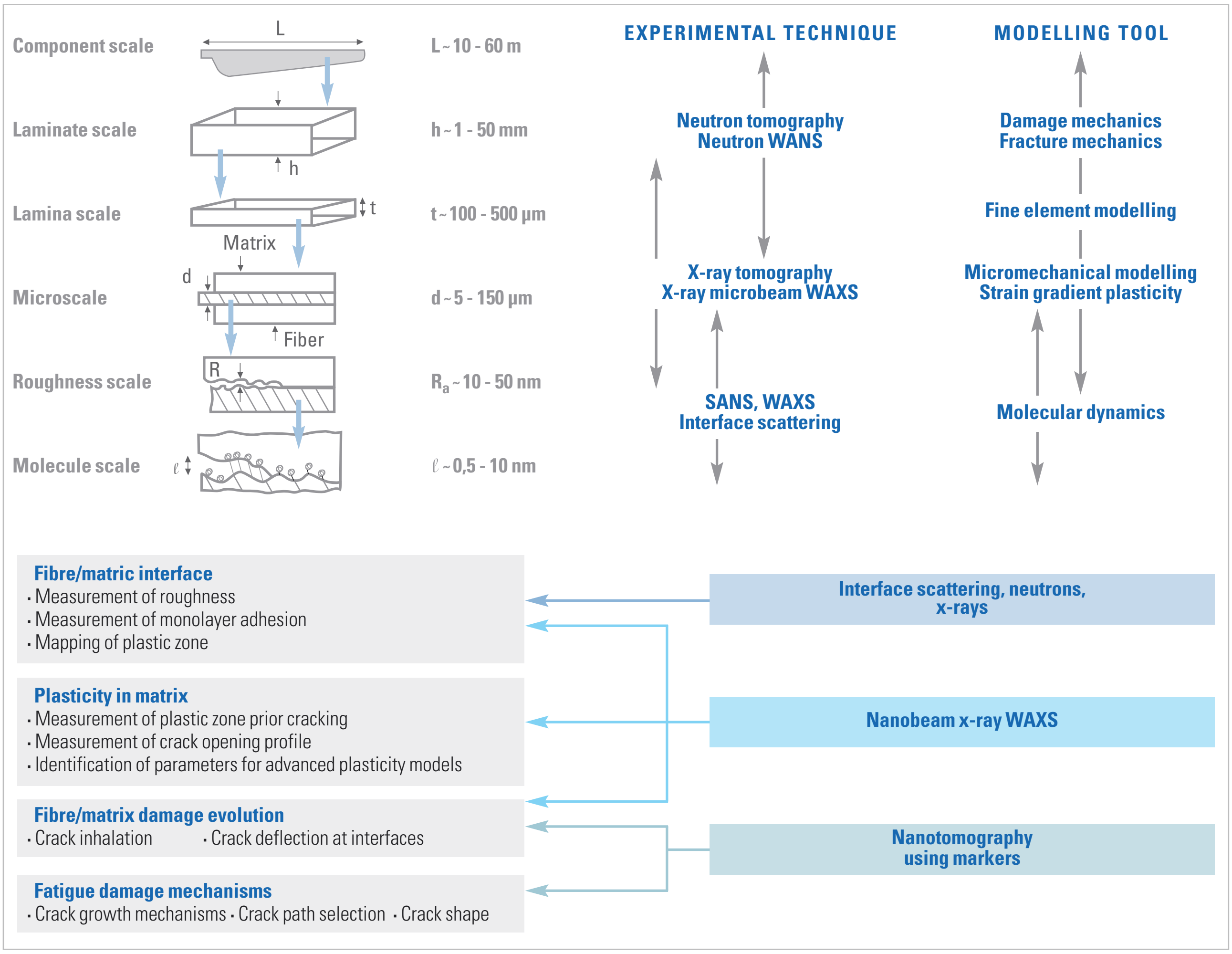


Fig. 11.3.9: An illustration of how damage propagation can be characterised.

lus, which can be used for through life monitoring when coupled to some computer or micro-processor. In this respect they are like functional materials providing some sensor capability: e.g. self diagnostic thermal barrier coatings with the thermal protection as primary function: thermal protection, but by incorporating i.e. thermographic phosphors into the coating one is able to independently measure bondcoat/TBC interface temperature, ceramic surface temperature and heat flux in-situ on rotating turbine hardware; all information needed for an engine thermal management system.

- **Intelligent nanomaterial systems**

The integration of smart nanostructured materials and functional surfaces into an intelligent material system: i.e. coupling smart oxidation/corrosion resistant coatings with a self-diagnostic TBC (Thermal barrier coating) both deposited onto a single crystal superalloy, with the smart coating providing the bondcoat. Piezo-spectroscopy and/or synchrotron radiation can be used to measure the strain in this alumina oxide, the self diagnostic TBC can measure the interface temperature and this combination results in a dynamic system to evaluate the creep life of the bondcoat and single crystal substrate. The surface TBC thermo-chromic sensing material permits to measure the ceramic surface temperatures and thus the susceptibility to CMAS attack, plus the interface and surface temperature permit heat flux to be measured thus permitting the optimisation of thermal loads.

The great challenge is integrating such systems into large industrial plants. Smart materials and intelligent systems provide future enabling technologies that cross many industrial sectors: construction industries, defense, agriculture, aerospace and power generation, environment, food and packaging, health care, space, sports and leisure, transport.

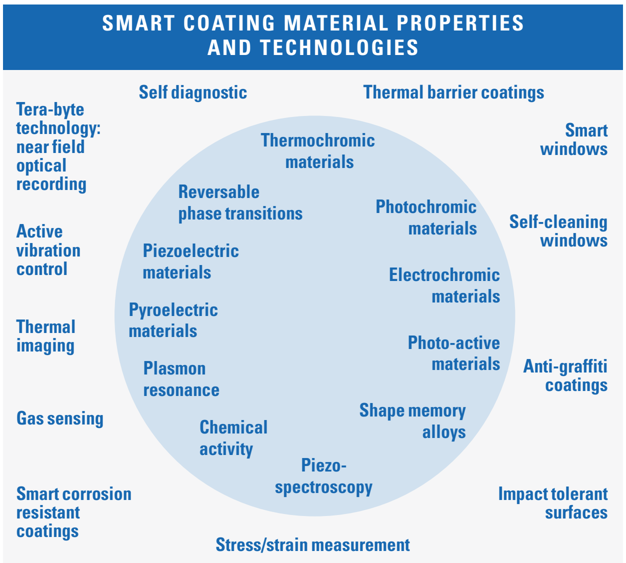


Fig. 11.3.10: Smart coating material properties and technologies.

11.3.14. CONCLUSIONS

Without a concentrated European activity it is unlikely that structural and functional nanomaterials will have sufficient critical mass and momentum to deliver radical new design concepts and step jumps in performance. One way forward is to bring together scientists, engineers and instrument scientists across both neutron and synchrotron platforms to create integrated Centres for Structural and Functional nanomaterials. This should be based around a 'hub and spoke' model linking scientists and facilities around Europe with a European Centres with facilities to manipulate nanomaterials (e.g. optical tweezers, nanofabrication and tooling) and instruments and capabilities for in-situ environments.

Researchers at many institutions throughout Europe may lack the expertise and/or the appropriate equipment for the synthesis and characterisation of new high-quality nanomaterials. European centres – embracing interdisciplinary approaches – are needed to provide a full suite of modern instrumentation, experimental facilities, computational and theoretical tools and expertise for nanoscience and engineering research.

The Euro-centres should provide a pathway from fundamental science, to applied engineering and to the creation of start-up companies. PhDs and staff member scientists should become familiar with basic science and user-support services.

European Centre for Advanced Synthesis and Processing

A major scientific challenge is how to synthesise or fabricate nanomaterials in which electronic, atomic, and molecular organisation varies spatially and temporally; so to understand principles and rules that govern the behavior of materials over different length and time scales.

Synthesis laboratories in Europe and worldwide have sufficient expertise/knowhow in the preparation of 1st and 2nd generation nanomaterials. The synthesis and processing of "smart" nanoparticles/materials with multiple functions ("3rd generation nanostructures") demand a European approach in which the role of synchrotron radiation and neutrons is of vital importance (see Figs. 11.3.11 – 11.3.12).

- Convergence of physical, chemical and biological synthesis techniques,
- In-situ characterisation under various environments (water, different gases, high pressure) and external electromagnetic fields (medical applications),
- Continuous control of the nanoparticle growth during all individual steps, and
- Synthesis modelling/simulation of complex hybrid nanoparticles and the interaction between them to achieve the optimal synthesis/processing methodology for the fabrication of complex hybrid nanoparticles.

European nanosynthesis laboratory operating at a large test facility

It is suggested to create a European laboratory in which a platform of off-line and on-line interdisciplinary synthesis clusters are available. Such a new European synthesis laboratory is necessary to keep Europe in a forerunner position for "synthesis-science" and "processing-industry" and will give Europe a competitive place in the global nanotechnology scene.

The primary focus of the nanosynthesis centre is on the design, the discovery and the advanced characterisation of new nanomaterials. It gives the possibility to move the experimental nanomaterials synthesis set-up in front of the beamline and to execute experiments in situ. This approach is of vital importance for the understanding of the mechanisms during synthesis and this will finally lead to the creation of new complex nanomaterial designs and give guidances to the fabrication of industrial nanomaterial fabrication processes.

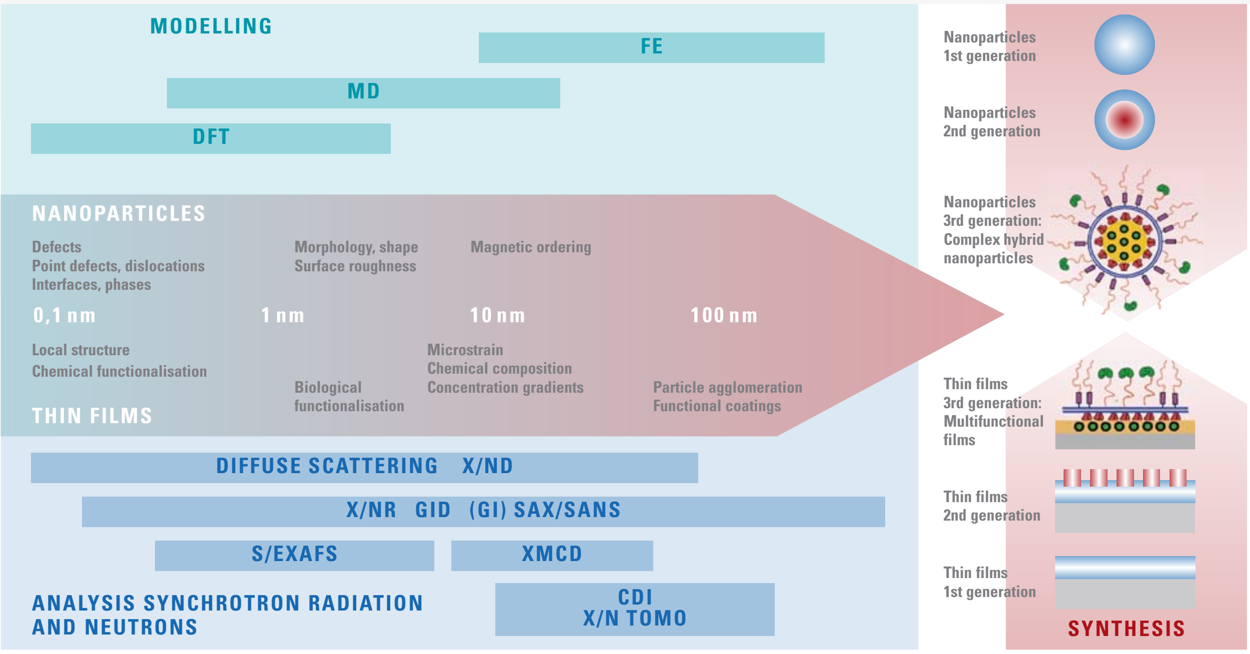


Fig. 11.3.11: Synthesis of 3rd generation smart nanometarials.

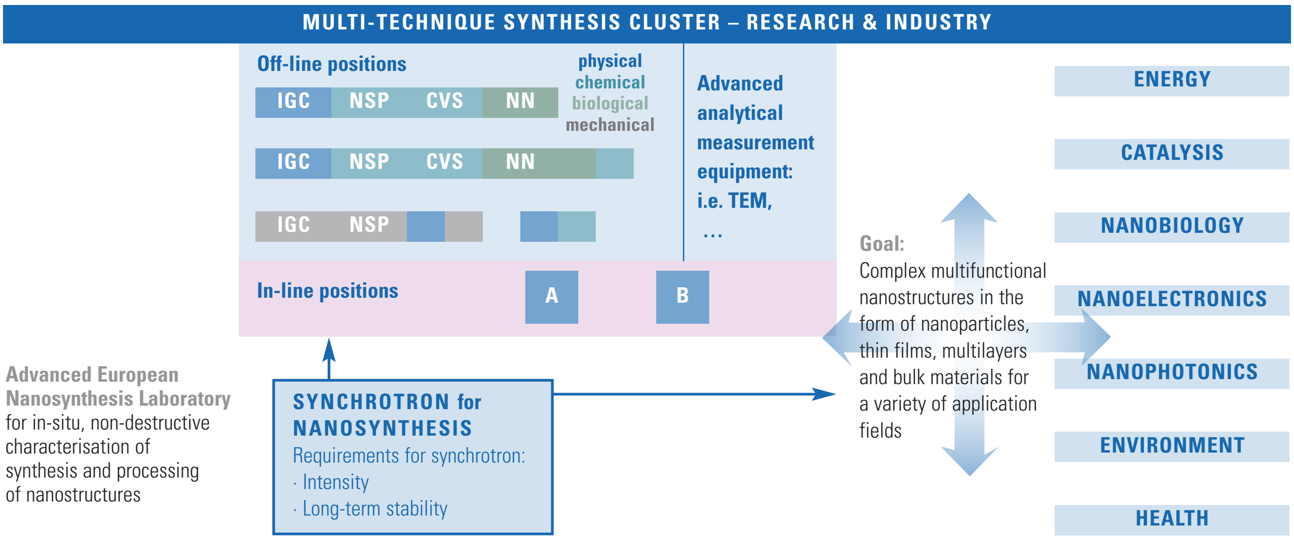


Fig. 11.3.12: European nanosynthesis laboratory installed at a large-scale test facility.

11.4. KEY CHALLENGES FOR NANOMATERIALS ENGINEERING

The design with nanomaterials is in its infancy. This chapter formulates the research, technology and development needs to reach the stage of reliable and environmentally-friendly engineering designs. The complexity of manufacturing and damage mechanisms are illustrated in Fig.11.4.1. To understand the mechanisms in processing, engineering, lifetime behaviour demands for qualitative- and quantitative understanding. This requires the use of synchrotron radiation and neutrons.

The engineering of nanomaterials covers a wide spectrum of applications ranging from nanoinformatics, bio-nanosystems and mechanical engineering: energy, transport and so forth. In order to reach breakthroughs in nanomaterials engineering, a partnership with universities, materials research centres, industry and experts at large-scale facilities is key. In order to ensure final success, the creation of a European research programme is necessary and a European Centre of Excellence in nanoengineering should be put in place.

11.4.2. OXIDATION/CORROSION HIGHLIGHTS

In-situ, synchrotron radiation-based studies under industrially relevant conditions (near atmospheric gas pressures/elevated temperatures or in corrosive solutions) on model systems (single crystal surfaces, vicinal surfaces with regular steps, nanoparticles with well-defined shape) give an atomic scale insight into (see Fig. 11.4.2):

- Complex structure and chemical composition of thermally grown oxide films;
- Interfacial structure and bonding;
- Growth mechanisms of protective layers for varying dimensionality;
- Oxidation/corrosion induced segregation and de-alloying;
- Catalytic activity of metal surfaces and nanoparticles under oxidation/reduction cycles.

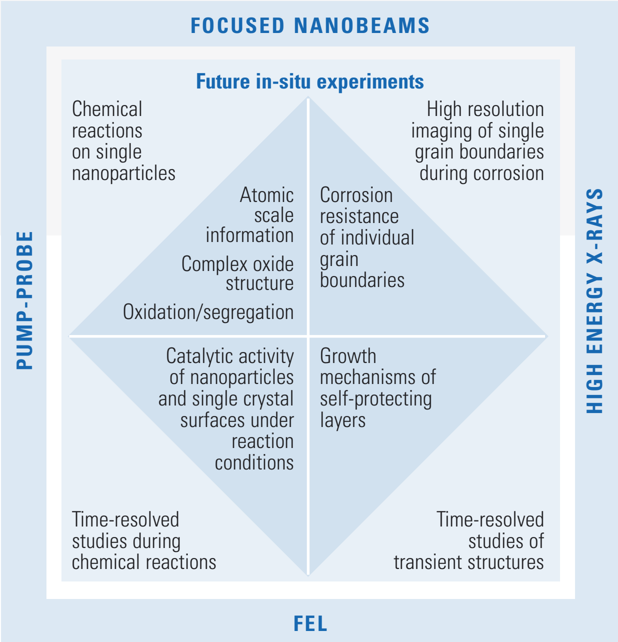


Fig. 11.4.2: Future in-situ experiments in the field of oxidation/corrosion.

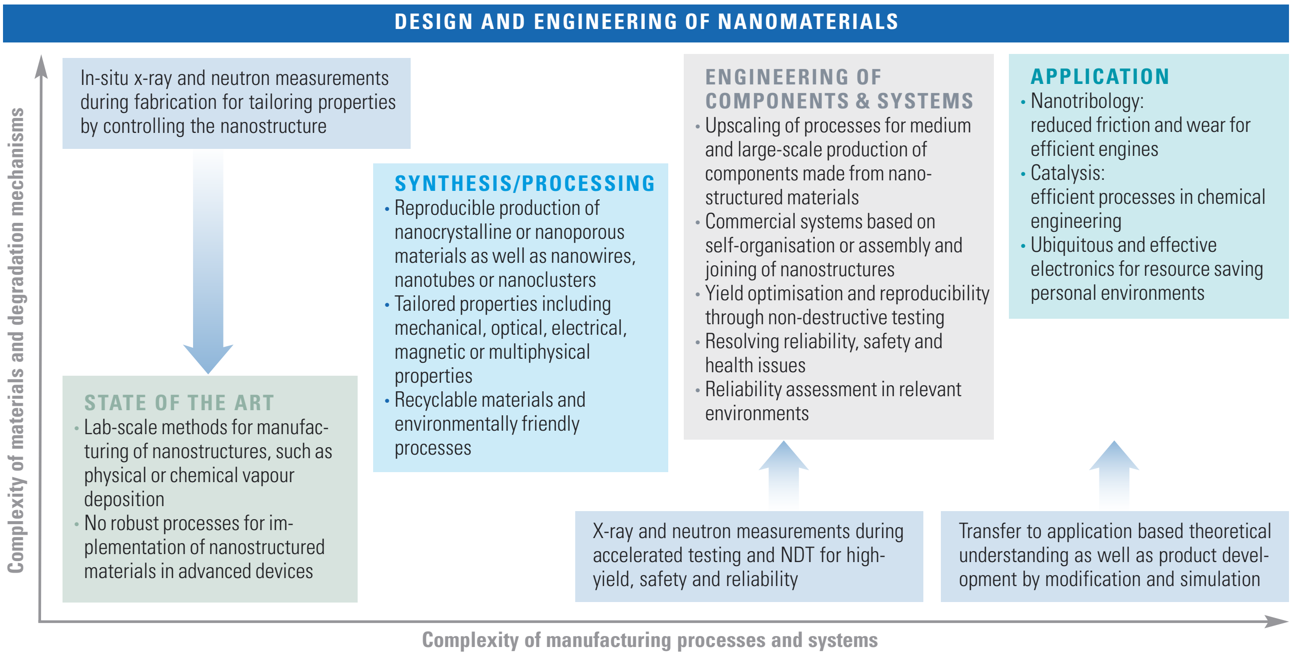


Fig. 11.4.1: Design and engineering of nanomaterials.

Furthermore, in-situ corrosion studies on polycrystalline, technically relevant materials using synchrotron radiation-imaging techniques give micrometre scaled information on:

- Corrosion resistance of different grain boundary types;
- Crack propagation during stress corrosion cracking.

Future breakthroughs:

- In-situ studies of large ensembles of identical nanoparticles under reaction conditions;
- In-situ studies on small ensembles or single nanoparticles using nanometre focused synchrotron x-ray beams;
- Time-resolved structural and spectroscopic studies during chemical reactions using ps x-ray pulses in pump-probe configuration (free electron laser);
- Time-resolved studies of transient structures during cyclic catalytic reactions and corrosion using high energy x-ray diffraction;
- In-situ tomography studies of grain boundaries under corrosion conditions using nanometre focused x-ray beams.

11.4.3. OPPORTUNITIES FOR NANOJOINING

The rapid development of nanomaterials research will only prove useful when the materials produced such as nanotubes, nanowires, nanostructured alloys and nanocomposites can form integrated parts of devices and components. In many of these applications, joining is foreseen to be an enabling technology. Special joining techniques and methods are required to achieve nanoscale electronic devices from CNTs, to enable NEMS assembly or to fabricate nanoscale smart structures devices with molecular sensitivity. The needs of product miniaturisation, of efficient and environmentally-friendly material utilisation are the key drivers of nanojoining development. The industrial potential of nanojoining is meaningful and involves molecular electronics, electronics and photonics, smart structures as well as structural applications. The development of novel joining concepts for nanomaterials will satisfy the current needs of business and society in regard to automotive, aerospace, chemical, energy, medical and microelectronics industries.

Main challenges associated with joining of nanomaterials that must be addressed are:

- Exploiting nanophenomena for new joining concepts;
- Understanding the joining processes at nanoscale to achieve controllable and consistent joints;
- Development of novel mass-production friendly processes (including suitable equipment) that do not destroy the carefully designed nanostructure;
- Development of new testing methods;
- Assembly process automation and materials handling.

Besides extreme challenges, the discovery of nanoeffects and nanomaterials brings a lot of opportunities for the joining technology. They are:

- Melting point suppression of nanoparticles which can be utilised to significantly reduce the joining temperature and to minimise thermal load during processes. "Cold" joining process that would be gentle to the nanostructured materials whilst joining can be theoretically developed;
- Higher reaction velocities for nanosized materials and shortened diffusion distances when using nanosized joining media which allow to reduce the processing time from hours to minutes or even seconds, turning the laboratory processes into potential industrial processes;
- The tendency of nanoparticles to stick to each other due to high surface areas what can be used to create self-assembled joints;
- The possibility to impart functionalities (thermal or electrical conductivity, mechanical enhancement or ease of disassembly and recycling) into a joint when using nanomaterials.

In order to succeed in the joining of nanomaterials, it is necessary to:

- Understand the behaviour of nanomaterials and structures along with their physical, chemical and biological interactions during and after joining from nano- to macro-scales (from 10^{-10} m to 10^{-8} m) and at different timescales from (10^{-4} s to 102 s);
- Develop multiscale computational models that can predict the performance of these nanostructures by considering the quantum effects as a function of composition, size and external field and support the development of nanojoining concepts;
- Develop nanoscale measurement devices which can sense the nanostructure architecture while processing and interrogate the nanostructures after processing are warranted.

Furthermore, a shift in engineering philosophy requesting a comprehensive treatment of joining in education and research needing has to proceed. Joining must turn into an integral part of primary processing, into a process which creates desired structures and is practised as much by physicists, chemists as by welders to take full impact on the development of nanomaterials. In the near future, nanomaterials synthesis and device production need to occur as an integrated and preferably simultaneous procedure.

The future of nanojoining can be envisioned in four distinct steps (Fig. 11.4.3). A close inter- and transdisciplinary cooperation between life sciences and engineering fields is required to reach the goals.

11.4.4. OPPORTUNITIES FOR NANOTRIBOLOGY

The tribological interactions of a solid surface's exposed face with interfacing materials and the environment may result in loss of material from the surface. The process leading to loss of material is known as "wear". In recent years, nanotribology has been gaining ground. Frictional interactions in small components are becoming increasingly important for the development of new products in electronics, life sciences, chemistry, sensors and by extension for all modern technology. The distinction between nanotribology and tribology is primarily due to the involvement of atomic forces in the determination of the final behaviour of the system. However, the statistical behaviour of the ensemble remains crucial and therefore we have to combine the atomic forces with the synchrotron radiation and neutron studies form the basis for the formulation of design criteria and codes of practice for nanotribology.

Synchrotron radiation and neutron studies form the basis for the formulation of design criteria and codes of practice for nanotribology. An overview of the research directions is given in Fig. 11.4.4, which also highlights the role of synchrotron radiation and neutrons in nanotribology.

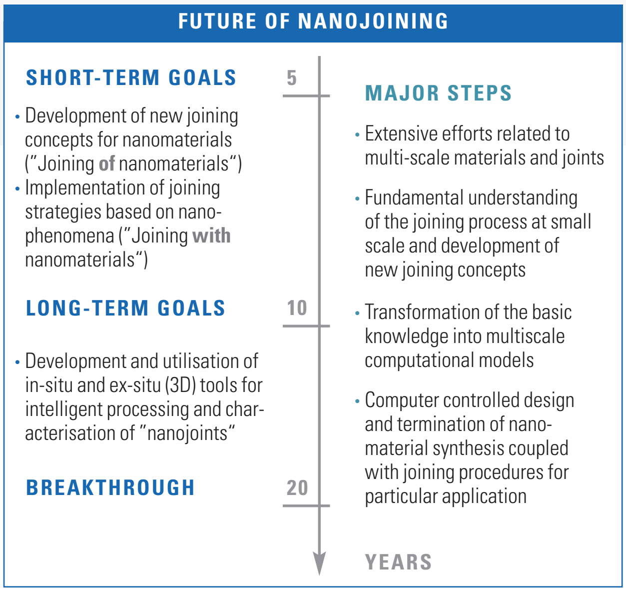


Fig. 11.4.3: Future of nanojoining.

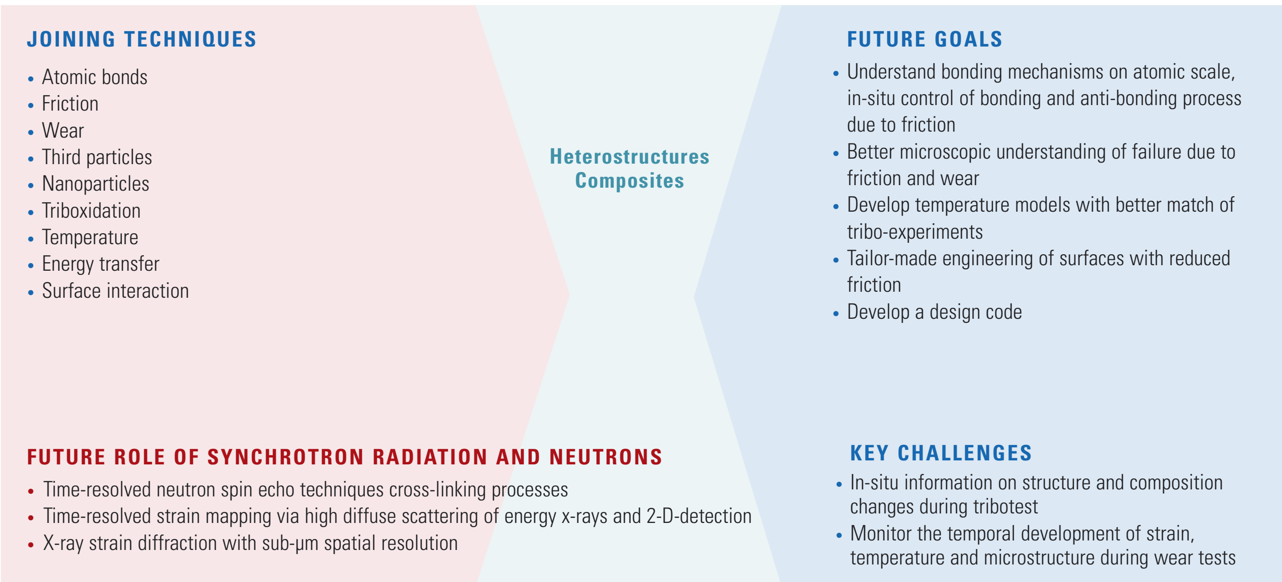


Fig. 11.4.4: Targets and challenges for research on nanotribology.

11.5. KEY CHALLENGES FOR NANOMATERIAL TECHNOLOGIES

11.5.1. OVERVIEW

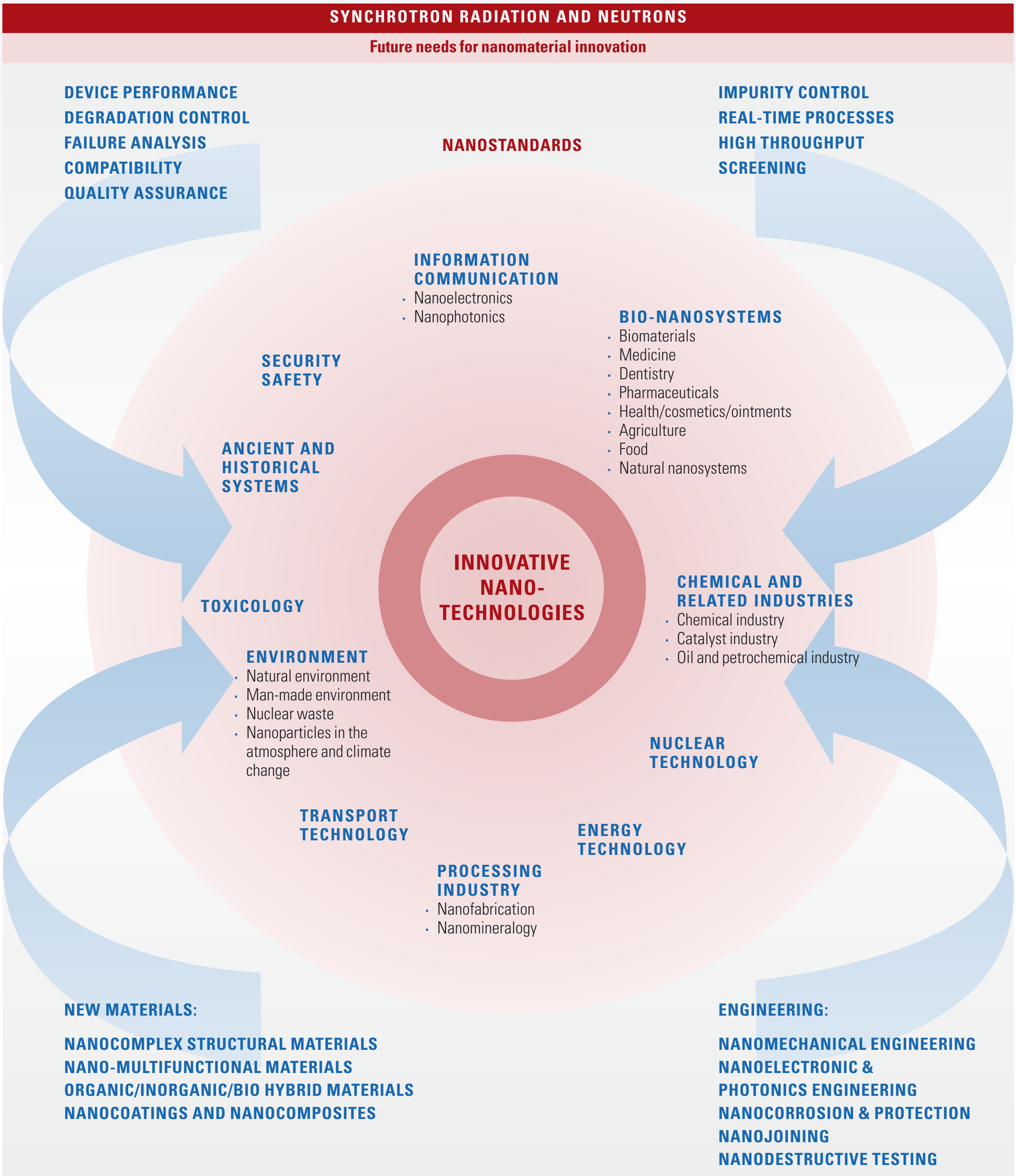


Fig. 11.5.1: Motivation of European research through the cycle of innovation and demand.

11.5.2. INFORMATION AND COMMUNICATION: NANOELECTRONICS AND PHOTONICS

Over the last decades, semiconductor-based electronics and photonics have made remarkable progress and revolutionised the way our society operates. During this time frame, silicon microelectronics technology exhibits an unstoppable pace of technology advancement. Currently there is a growing concern about whether semiconductor technology can continue to keep pace with demand when microelectronics and photonics industries enter the "deep nanoscale" dimension. Large synchrotron and neutron sources provide unique characterisation tools for the complex materials involved in advanced microelectronic and photonic devices. Their role in the development of future nanoelectronics and nanophotonics industries will be of vital importance for achieving prospective breakthroughs.

Potential developments in nanoelectronics

The physical limits of downscaling CMOS technology will be reached towards the end of the next decade, and the further developments of nanoelectronics are so far in the state of basic research. Three new scenarios are forecast for the short, medium, and longer term future, in order to develop new technologies:

- "More Moore": To further improve the performance enhancement by effective downscaling processes: continuation of Moore's law to cope for modern world's demand of faster, smaller, cheaper and more efficient information technologies;

- "More than Moore": to add new functionalities to current integrated circuit technologies;

- "Beyond CMOS": to open completely new directions like spintronics and molecular electronics with new concepts. (Beyond CMOS) and for developing new information processing technology after CMOS.

An overview of the potential developments in nanoelectronics beyond the CMOS technology is presented in Fig. 11.5.2.

To achieve the objectives, the research needs to include bottom-up approaches, new materials with specific functionalities and special processing architectures are highlighted:

- New materials for ICs: high-κ dielectrics for gate insulators, low-κ materials for interconnects;
- New device structure for electronics: 3D-integration, nanowires and carbon nanotube-based electronics;
- Logic devices: single electron transistor, molecular switches, magnetic transistor;
- Memories with new architecture concepts: resistance-based memories, electronic effects memories, macromolecular and molecular memories;
- Spintronics: hybrid electronic, optical, and magnetic systems, spin coherence elements;
- Molecular and organic electronics: hybrid electronic-biological systems;
- Quantum state logic and computing.

A micro- and nanoelectronic device generally consists in gathering logic switches (transistors) and memories (DRAM, SRAM, flash) for storing and delivering information. In the **"More than Moore"** concept transistors and memories are integrated either on the same chip; 3-D integration or assembled in the same package (Fig. 11.5.3). The challenges in materials research and development strongly depend on the constitutive device parts where nanomaterials are integrated: transistors, memories and packages.

Challenges in nanoelectronics

The main challenges in the development of nanoelectronics are related to:

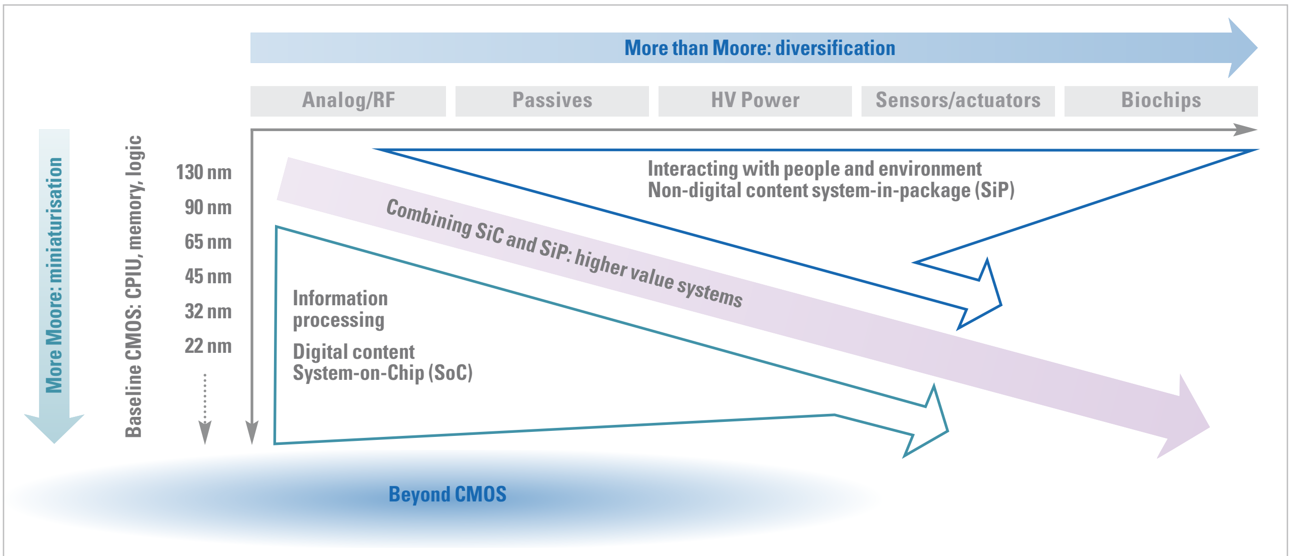


Fig. 11.5.2: Moore's law and More than Moore concepts.

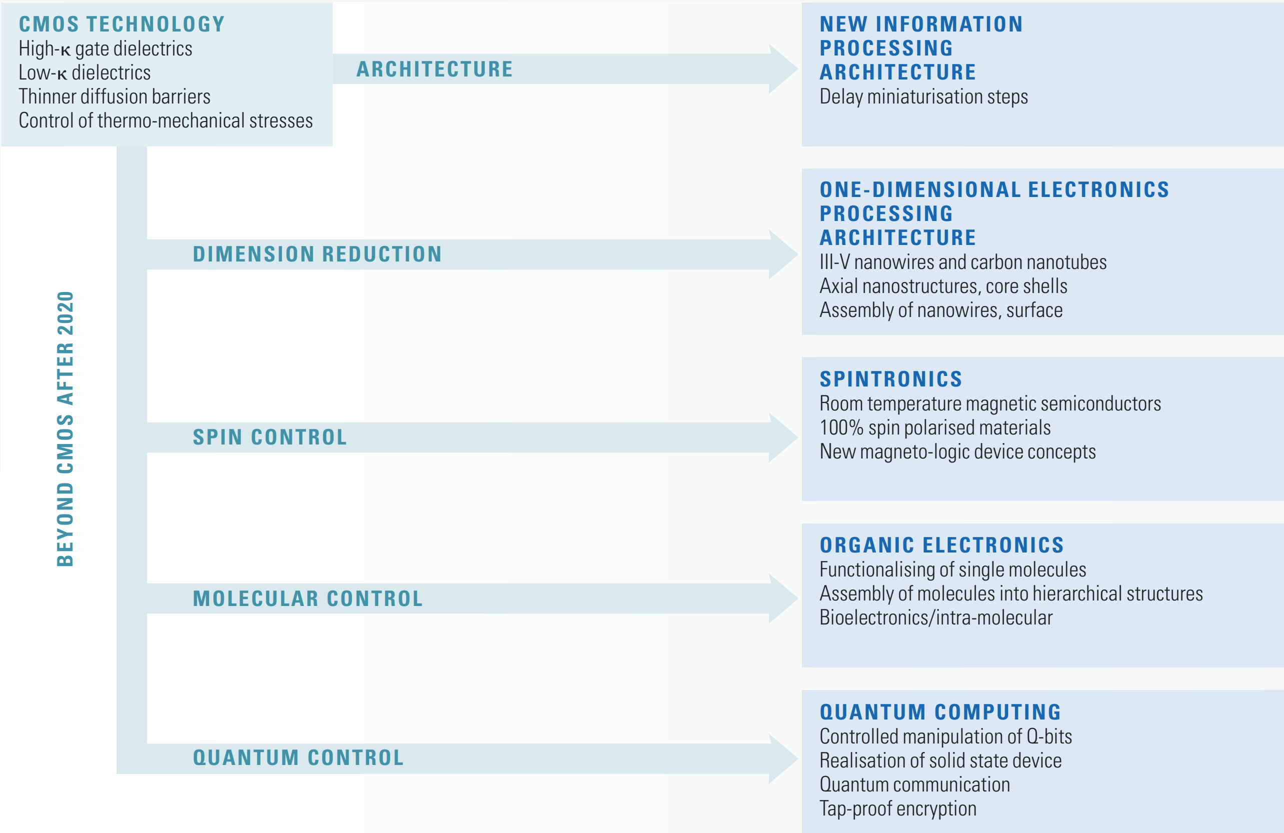


Fig. 11.5.3: Development of nanoelectronics: More Moore and Beyond CMOS.

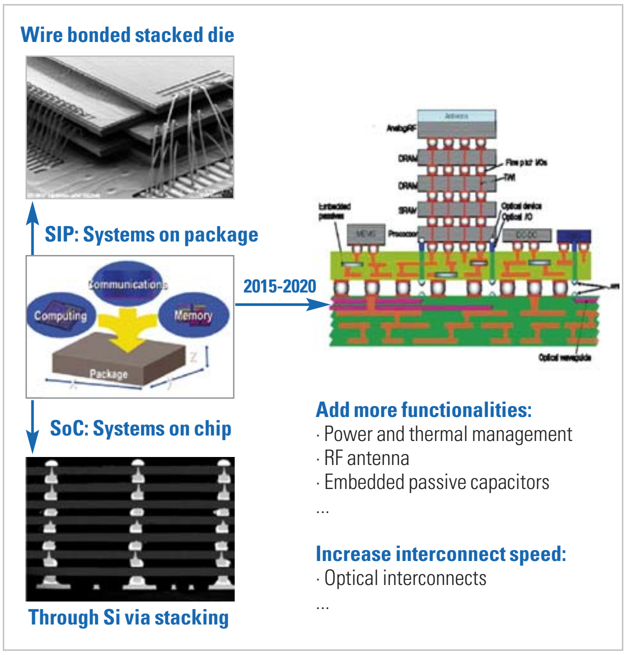


Fig. 11.5.4: Development of nanoelectronics: More than Moore.

- **Device Miniaturisation (More Moore):**
  - Multiple gate FET;
  - Enhanced CMOS channel mobility;
  - Control of the high κ-metal gate stack;
  - New materials for improving metal conductivity and lowering interconnect dielectric permittivity.

- **Integration of new functionalities (More Than Moore)** (Fig. 11.5.4):
  - Integration of sensors with ICs;
  - Integration of actors;
  - Integration of biological elements.

The 3-D integration starts with the integration of DRAM memories on a logic chip and by the integration of imagers over CMOS devices. Additional values will be available to the end-customer thanks to the integration of RF communications, power control, passive components, physical, chemical and biological sensors and actuators.

The main challenges of the More than Moore concept are related to the integration of more and more components at the 10–100nm scale, power management, electrical and thermo-mechanical reliability and

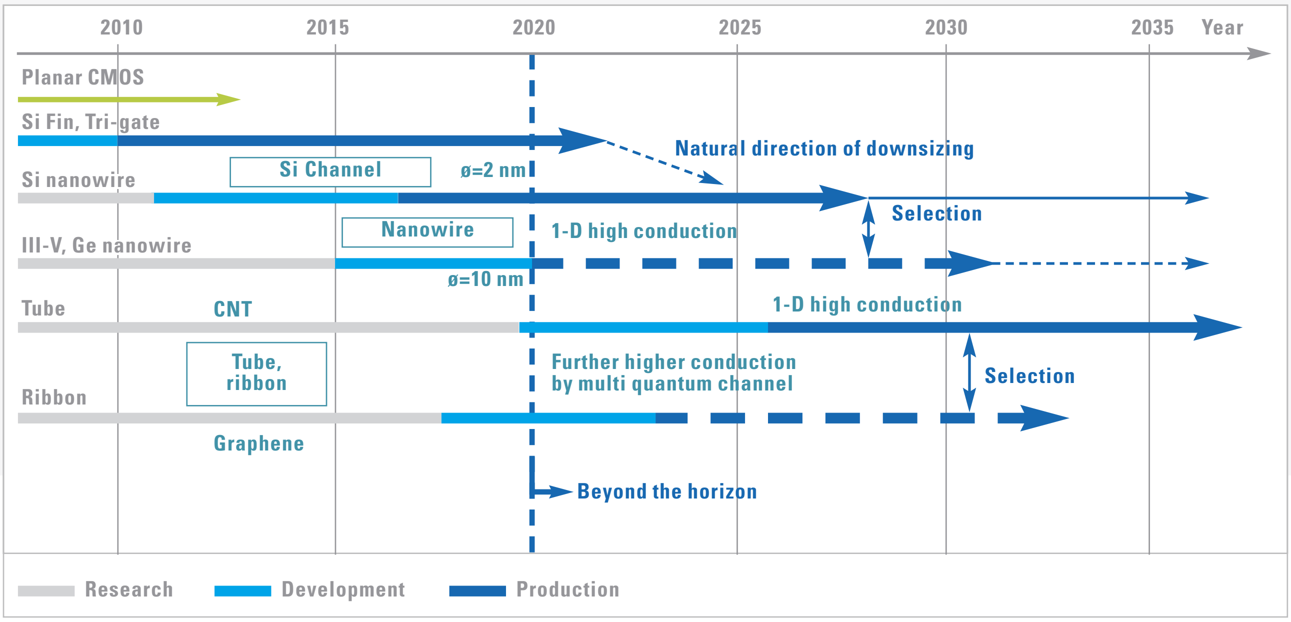


Fig. 11.5.5: R&D on materials related to the Extended CMOS transistor roadmap.

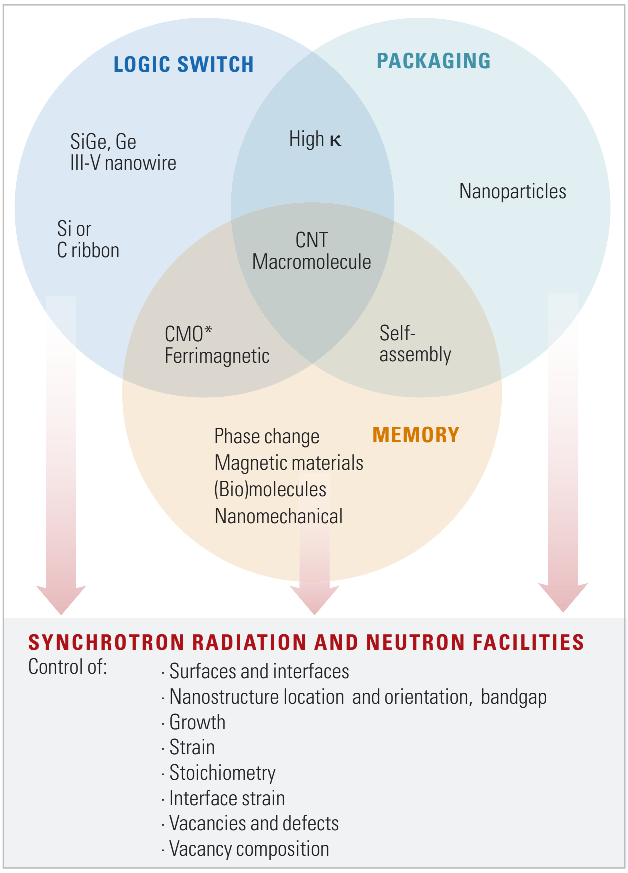


Fig. 11.5.6: Materials involved in nanoelectronics and the potential impact on synchrotron radiation and neutron facilities.

increase of the metallic line length. The increase of interconnect length will naturally slow down the signal propagation between the various components.

- **Beyond CMOS**

The "Beyond CMOS" approach, emerging devices will not substitute the CMOS transistor before 2025–2030, unless a considerable breakthrough occurs within the next 10 years:

- Single electron transistor for threshold logic devices;
- Molecular switches;
- Ferromagnetic transistor.

In terms of materials R&D the main challenges are depicted in Fig. 11.5.5.

Advanced non-volatile memories require specific R&D activities in order to overcome the great challenges related to enhanced integration density. This development will involve new concepts and new nanomaterials such as:

- Ferroelectric polarisation;
- Ferromagnetic transition metals;
- Magnetic polarisation: materials for spintronics;
- Resistance change: complex metal oxides;
- Nanomechanical memory: low dimensional materials;
- Molecular memory: macromolecules;
- Biomolecular memories.

The key challenges related to the development of these memories are described in Fig. 11.5.6, illustrating also the role of synchrotron and neutron facilities to overcome them.

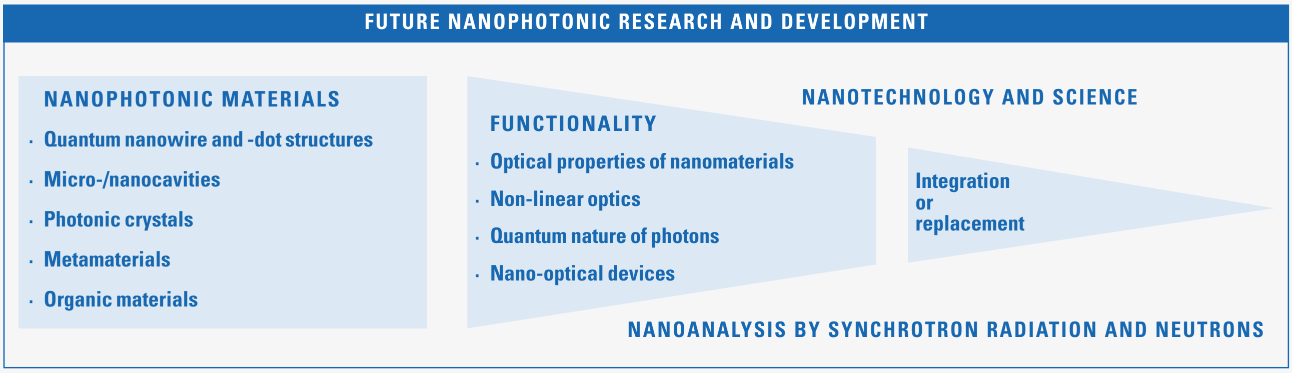


Fig. 11.5.7: Nanophotonics roadmap.

Potential development of nanophotonics

The focus lies i) on the integration of novel photonic devices into existing electronics, or ii) to replace electronic by photonic components. Nanophotonics consists in mastering and shaping optical fields at scales that are quite lower than the light wavelength for developing new optical and opto-electrical devices. The main applications of nanophotonics concern telecommunications, displays, sensors, data storage, biomedical imaging, vision systems, and optical interconnects.

The nanophotonics developments are strongly coupled to new photonic materials and nanotechnologies:

- Quantum wires and dots in Si, III-V and II-VI materials for data storage, lighting and optical interconnects;
- Plasmonic structures for sensors and imaging devices;
- High contrast Si and III-V nanostructures for telecommunications, biomedical imaging and lighting;
- Organic nanostructures and carbon nanotubes CNT for displays;
- Nanoparticles in glass and polymers for optical interconnects and telecommunications.

Nanophotonic component developments use different kind of materials and substrates: II-VI, III-V compounds, silica, glasses, fibres, and organic materials to be applied as lasers, photo-detectors, multiplexers. Fig. 11.5.7 highlights the future nanophotonics research and development phases.

The mass-production of microelectronic devices on large silicon substrates considerably reduces the cost of each individual device and improves its performance reliability; so, the interest to "siliconise"

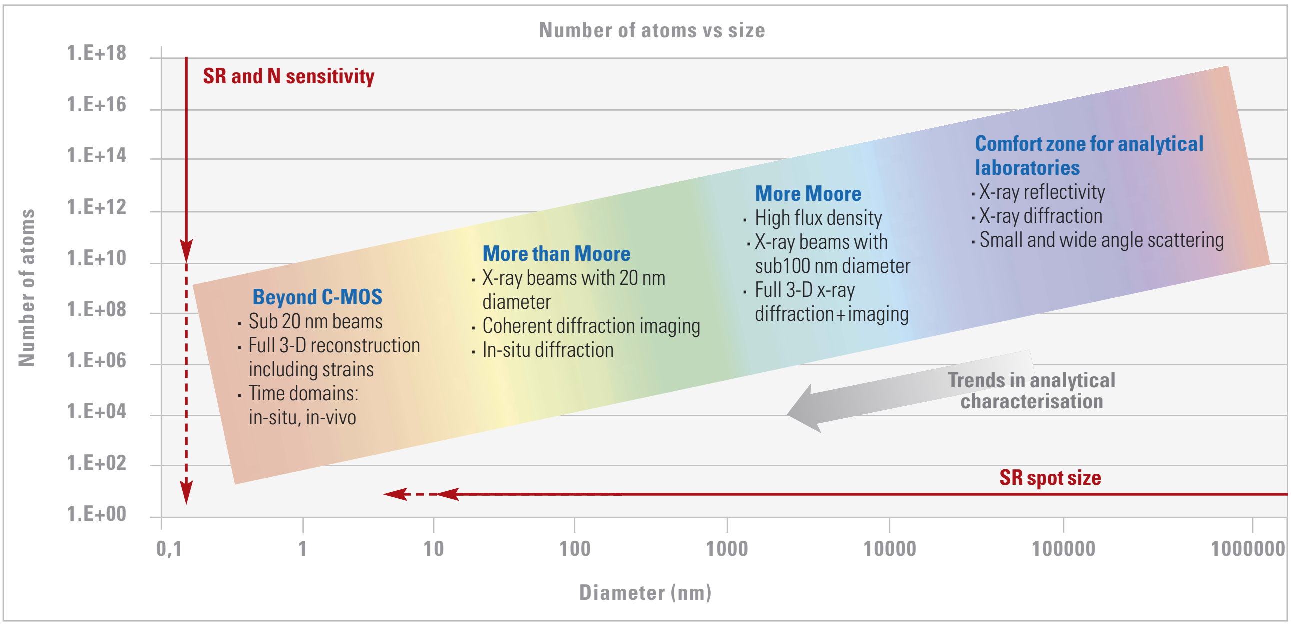


Fig. 11.5.8: Analytical challenges: nanoelectronics.

photonics is strong for achieving rapid progress in the nanophotonics field and competitive prices. Consequently, nanophotonics and nanoelectronics should converge soon. Silicon nanophotonics will not be easy because silicon does not exhibit convenient optical properties for realising laser sources and detectors.

Nevertheless, since empowering silicon with optical functions (such as the ability to emit, guide and modulate light) can be the key for creating short-distance ultrafast optical interconnects allowing to scale the speed of computing, nanophotonics will essentially be developed on silicon chips.

The developments in nanophotonics on silicon will focus on the production of a source of photons (quantum dots, nanostructured Si,…), electro-optic modulator, photodetector. The characterisation of strain, surfaces, interfaces will be fundamental for the development of nanophotonics.

Characterisation requirements: synchrotron and neutron sources

Future successes in nanoelectronics and nanophotonics era critically depend on the discovery of alternative materials and on the introduction of novel types of functionalities and information processing architectures (see Figs. 11.5.1 – 11.5.7). This unambiguously requires dedicated characterisation of new material properties at the nanometre scale, and here synchrotron and neutron radiation will play a key role:

- Small **nanosized probe** volume to quantitatively analyse structure, chemistry, electronic and magnetic properties of nanomaterials with high spatial resolution and high sensitivity;
- Non-destructive **three-dimensional (3-D) reconstruction** of singular nano-objects ("3DXRD") for studying shape, surface, subsurface and interfaces, defects and direction-dependent physical properties; i.e. thermo-mechanical stresses in real devices;
- **In-situ characterisation** to study the structural-electronic-magnetic phase transitions in nanomaterials and time-dependent mechanisms (e.g. spin transport, spin dephasing).

In order to be able to carry out these kinds of measurements, the following qualifications have to be fulfilled for synchrotron and neutron facilities (Fig. 11.5.8):

- **High brilliance: high flux density:** for individual nanostructures (small and dilute samples), ability to penetrate coatings, fields, environments;
- **High momentum resolution: high spatial resolution:** for surfaces and interfaces, quantitative analysis of structure, strain, imaging;
- **Energy tunability: element specificity:** for the analysis of sensitive trace elements and chemical states, study of heterogeneous systems;
- **Time domain: in-situ AND in real-time:** for time-dependent processes, reactions.

Conclusions

Further developments in nanoelectronics and -photonics will have important impacts on the society. Research in this field is certainly a key to gain and/or maintain a leading position of Europe worldwide, with important impacts on the European economy and job market. Synchrotron radiation and neutron facilities will within these research efforts provide breakthroughs in the following research areas:

Fundamental research

- Small and wide angle scattering for a full 3-D analysis of complex nanostructures;
- Multiscale analysis: determination of properties from atomic scale up to grain level using micro- and nanofocused x-ray beams;
- Characterisation and understanding defects (generation, diffusion, segregation, thermal strain-induced, etc.);
- Study of local chemical environment (EXAFS);
- Combination of imaging and diffraction, model-free data analysis using coherent scattering and phase retrieval;
- Quantitative measurements of chemical bonding across hetero-interfaces, e.g. between dielectric, semiconducting, and metal films (UPS/XPS);
- Improved detection of hydrogen by neutron scattering and tomography in silicon devices.

Manufacture control/applied research

- Development of standardised x-ray/neutron reflectometry technologies for nanometrology of thin films and multi layers (thickness, density and interfacial roughness);
- Control of grain size in metallic interconnects;
- Control of the pore size distribution in low-κ layers by standardised small angle scattering beam lines;
- Routine measurement capabilities of texture in poly-crystalline films;
- In-situ and in-vivo control of device structures during fabrication and operation.

Future innovation in nanoelectronics and nanophotonics relies on the efficient cooperation of the involved parties: research institutes, universities, industrial laboratories, and large synchrotron and neutron facilities (see Fig. 11.5.9).

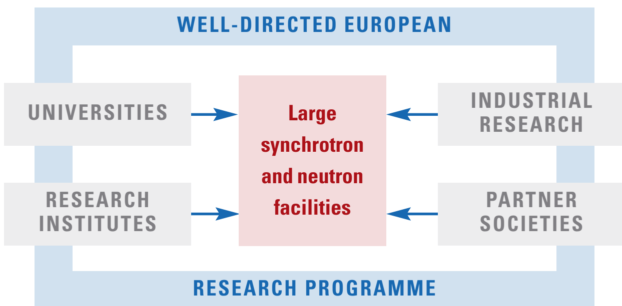


Fig. 11.5.9: Philosophy for a European research strategy and programme.

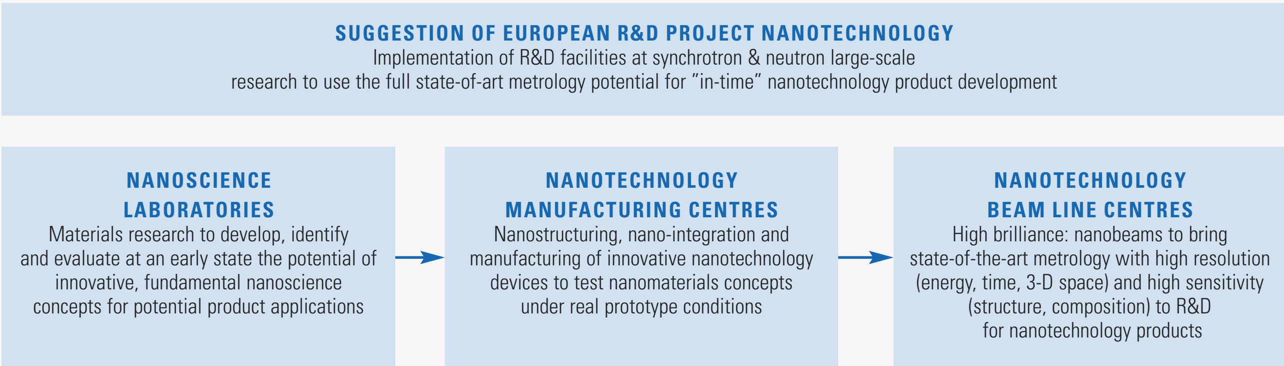


Fig. 11.5.10: Vital implications for a European research programme.

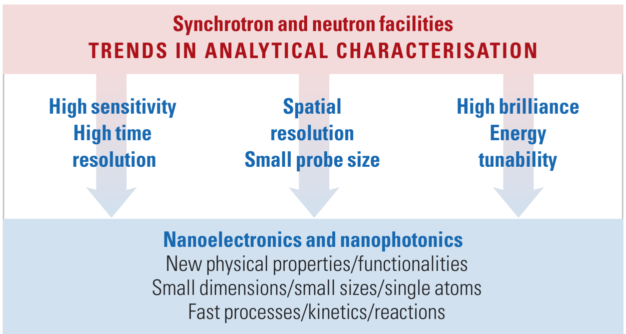


Fig. 11.5.11: Compulsory evolution of the analytical characterisation andits impact on synchrotron and neutron characteristics I.

For Europe to maintain a forerunner's position in nanoelectronics and photonics technology, a reputable and well-defined European research programme should be put into place (see Fig. 11.5.10).

In order to achieve this, a compulsory evolution of European synchrotron radiation and neutron facilities will be imperative for the scientific community (see Fig. 11.5.12) and the nanoelectronics and photonics industry (see Fig.11.5.11).

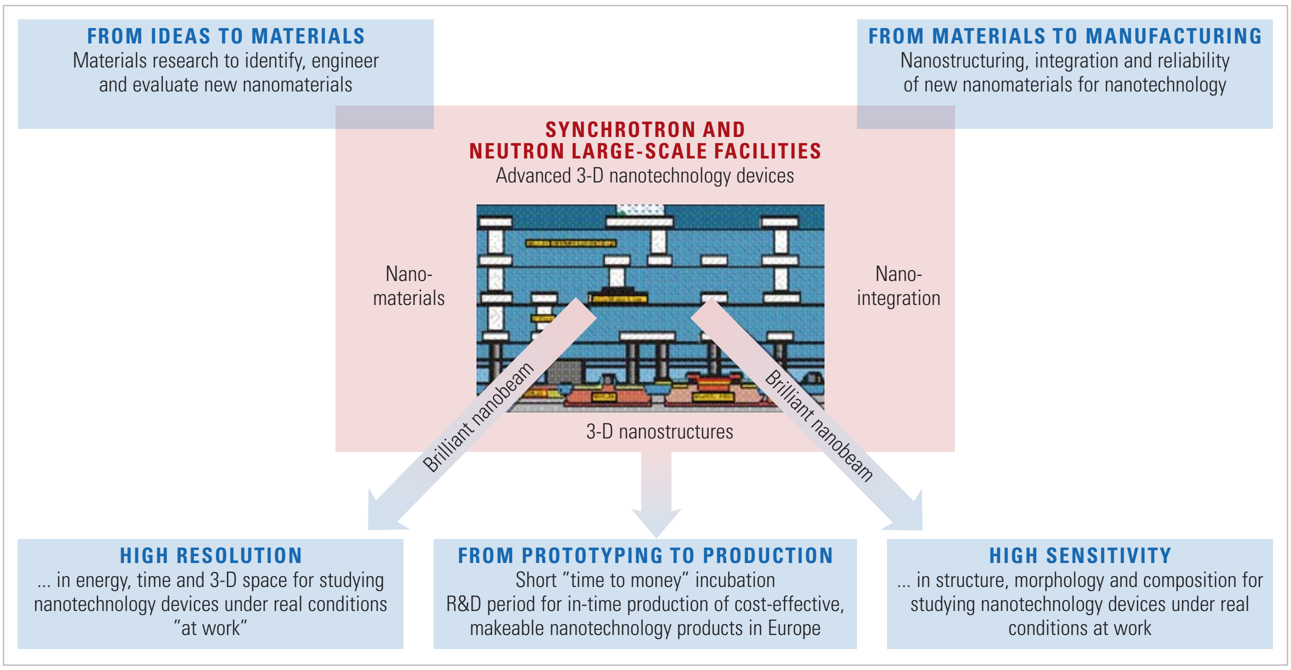


Fig. 11.5.12: Compulsory evolution of the analytical characterisation and its impact on synchrotron and neutron characteristics II.

11.5.3. BIO-NANOSYSTEMS

Bio-nanotechnologies relate to the interface between organised nanostructures and biomolecules which is the key control route for achieving new breakthroughs in medicine, dentistry and therapeutics, in food of animal and vegetable origin, and in products of daily care such as cosmetics. On the other hand, there is also the potential for toxicity, with associated risks to patients, consumer and the environment. Fundamental research and development on bio-nanopolymeric materials in particular, will greatly benefit from the additional structural, chemical and electronic insights into polymeric and living systems at the nanoscale which are uniquely offered by synchrotron and neutron facilities (see Fig. 11.5.13).

Research topics with synchrotron radiation and neutrons impact

- **Biomaterials** (see Fig. 11.5.14)
- Nanoparticle interactions with molecular, supra-molecular and cellular scale components of biological systems;
- Bioactive nanomaterials and therapies with controlled drug release and degradation;
- Functional derivatisation of the nanosurface and bulk material: systematic development of reproducible, well-characterised nanoparticles with traceable links to biological activity e.g. antimicrobial surfaces;
- Controlled degradation of biomaterials;
- Nanoparticle self-organisation and aggregation in biological systems;

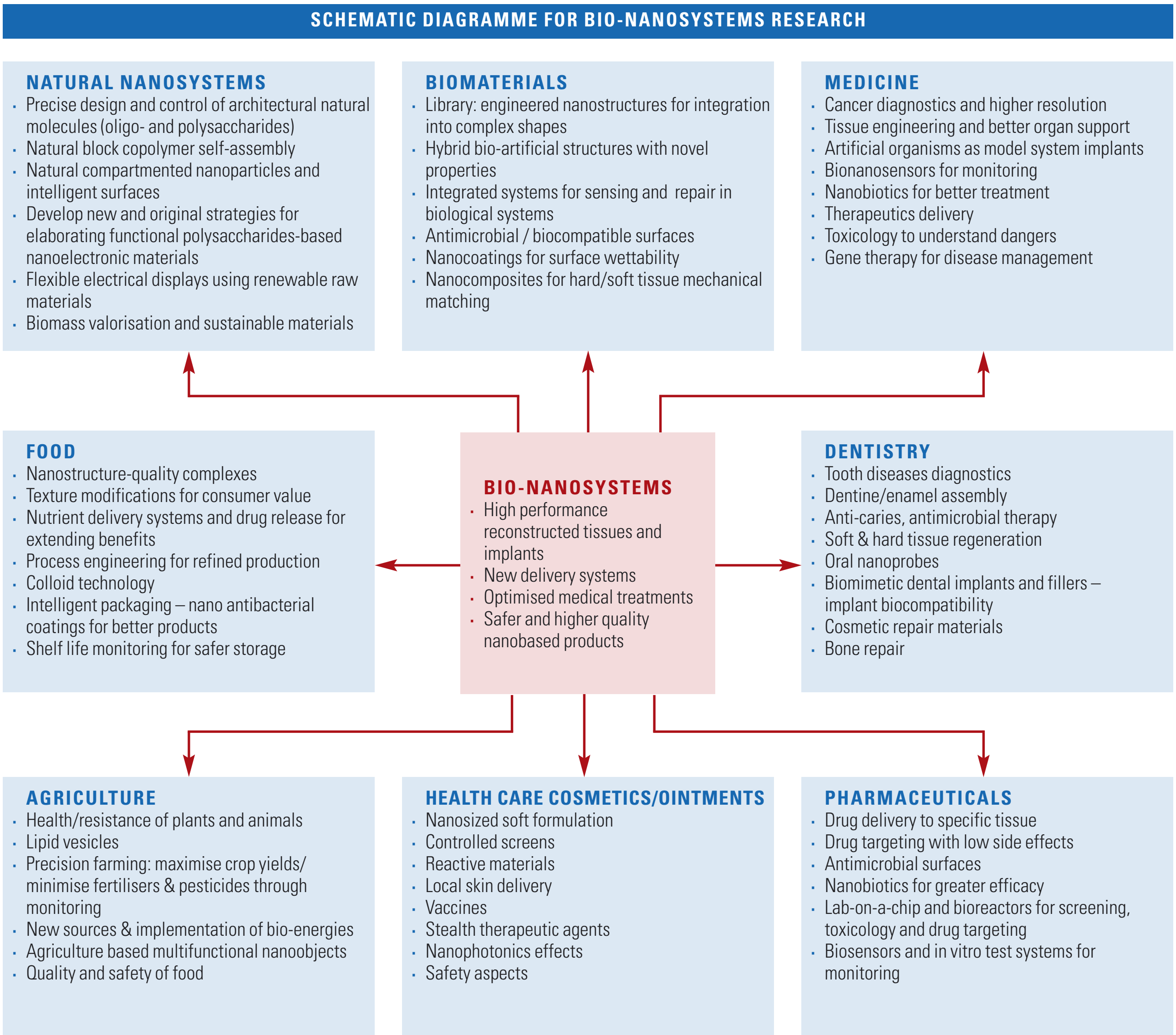


Fig. 11.5.13: Overview of bio-nanosystem technologies.

- Analysis of core-surface interrelationships;
- Asymmetric porous biomatched architectures to be fabricated;
- Solid and core-shell particles as vehicles for biological and therapeutic payloads;
- Cell and tissue guidance in microdomains for organ regeneration;
- Nanoscale sensing for 'intelligent' implants in clinical use;
- Mechanical adaptation of nanocomposites to be used as a route to biomimicry;
- Correlation between nanocomponent properties and macroscale implant constructs;
- Predictive modelling of in-vivo nanoparticle life cycle (uptake, activity, trafficking, disposal).

Synchrotron radiation and neutron facilities are needed for:
- Interrogation of surface structure and organisation at nanoparticles;
- Understand the organisation of water at the interface;
- Track protein, cell membrane and colloid surface interactions;
- Structural remodelling at the nanointerface;
- In-vivo tracking of nanoparticle-traffic;
- Engineering nanocomposites and their response to environmental and mechanical change;
- High resolution cell and tissue imaging;
- Target methods for precision therapy;
- Interrogating nanoscale structures of crystalline and amorphous nanoscale domains;
- Characterisation of chemical and structural features.

- **Medicine** (see Fig. 11.5.15)
  The applications of nanoscience and technology to medicine will benefit patients by providing new prevention assays, early diagnosis: nanoscale monitoring, and effective treatment via mimetic structures. Potential research areas are:
- Systematic studies of nanoparticle surface-biological colloid interactions for the design of biocompatible materials are needed. Better understanding of surface bio-compatibility microscopic understanding of surface interactions for improved surface design;
- Tissue substitute materials need to be based on nanoscale 3-D structures with controlled porosity and architecture. Orientation of biopolymers to control mechano-biological properties.
- Nanobiosensors need to be developed for early diagnosis;
- Multifunctional engineered nanostructures with controlled surface and bulk properties for sensing and targeted transport across in-vivo barriers: epithelial cell membrane or cell organelle for selective therapeutics require to be produced;
- Nanostructures for augmentation of imaging and conventional therapy (viz radiotherapy for cancer);
- Extracellular scaffolds for organ/tissue (e.g. liver, kidney, nerve) architectures for multicellular functional integration and to create viable replacement organs. Mimicry of natural architectural arrangements of tissues with regard to nanoscale orientation and multiplexing of extracellular polymers. Controlled scaffolds for self-assembly of tissue architectures as the basis for organ regeneration incorporating complex tissue architectures.
- Construct nanomachines for cell and tissue repair at both molecular and cell organelle levels;

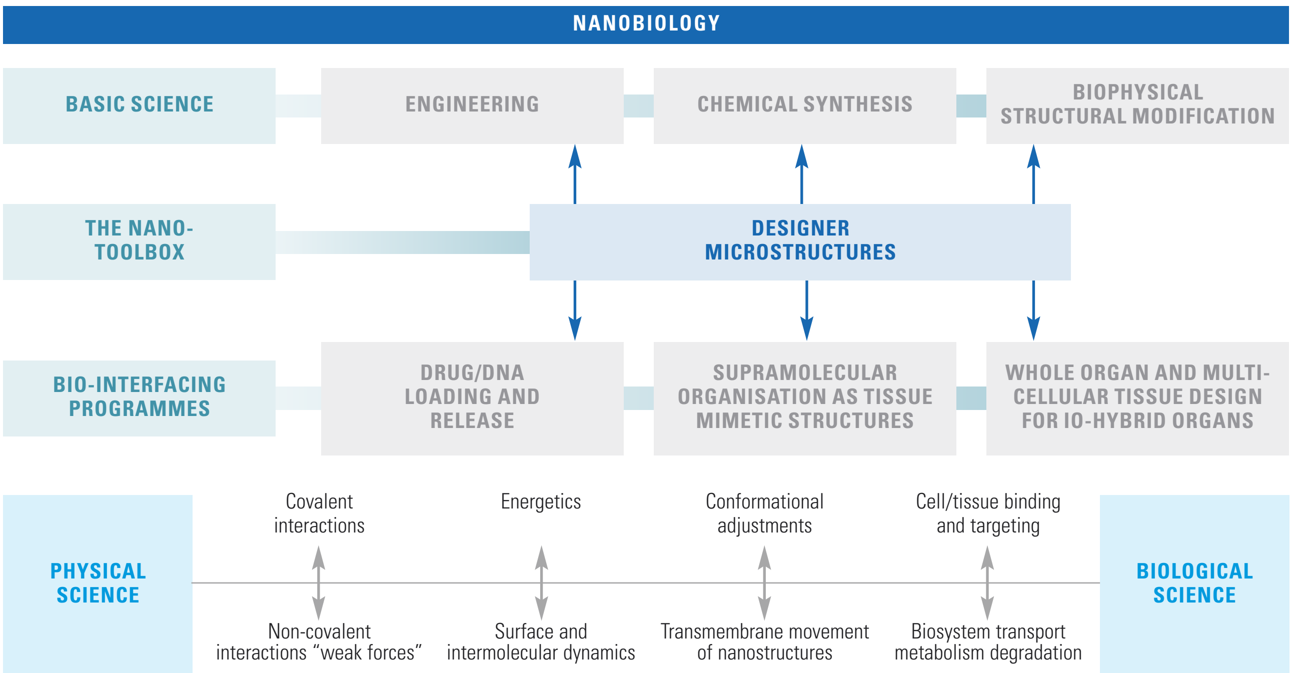


Fig. 11.5.14: Overview of bio-nanomaterials systems.

- Cell biology studies for correlating nanostructure interactions in the cell, the tissue matrix and intact tissue;
- Surface functionalisation of nanoparticles for chemical and physical environmental sensing, coupled with non-invasive techniques for registering their response. Systems for continuous multi-site/multi-organ monitoring for both pre-symptomatic diagnosis and early therapy need to be generated.
- Nanostructure design for mimicking viral and other natural particles to deliver drugs, gene therapies and cell repair systems to selected tissues; a vital area for traversing natural tissue barriers;
- Nanoparticle trafficking and disposal need to be understood in order to be able to harness such materials clinically;
- Controlled drug release (tissue location, kinetics);
- Develop intelligent nanostructure interfaces for distributed in-vivo monitoring and 'microscopic' tissue repair: high resolution tissue imaging;
- Monitoring and high level modelling of physiological systems;
- Nanomarkers i.e. gold particles in brain tumors for enhanced medical imaging.

Synchrotron radiation and neutron facilities are needed for:
- New selective imaging techniques at nanometre resolution for diagnosis and toxicology;
- Characterisation and imaging of chemical and structural features;
- Development of miniature devices for in-situ sensing and/or treatment;
- Improvement of drug targeting and delivery using nanoscale vectors for increase of effectiveness;
- Development of photo-activated radiotherapy with nanoparticles acting as enhancers;
- Dynamic functional radiography with specific synchrotron contracts enhancement;
- Radiation source for activated phototherapy;
- 2-D and 3-D imaging of composite nanostructured implants;
- Nanoscaffold-based tissue engineering;
- Synthesis of new functional and "intelligent" nanomaterials for long-term treatment.

Initiative for the Creation of a European Centre for Nanomedicine: "Opportunities offered by synchrotron radiation and neutrons"

Nanomedicine will improve healthcare in all phases of the care process. Synchrotron radiation and neutron sources will have a critical role in developing new diagnostic and therapy tools. New in-vitro diagnostic tests will shift diagnosis to an earlier stage, hopefully before symptoms really develop and allow pre-emptive therapeutic measures. In vivo diagnosis will become more sensitive and precise thanks to new imaging techniques and nano-sized targeted agents. Therapy could be greatly improved in efficacy by using targeted and minimally invasive synchrotron radiation and neutrons beams.

Visions for a European Research Programme: "key challenges"

1. Disease diagnosis (Fig. 11.5.16)

- Nanotechnology could improve in-vitro diagnostic tests by providing more sensitive detection technologies or by providing better nanolabels that can be detected with high sensitivity once they bind to disease-specific molecules present in the sample;
- Nanomedicine may permit earlier detection of a disease, leading to less severe and costly therapeutic demands, and an improved clinical result. Conceptually novel methods, combining biochemical

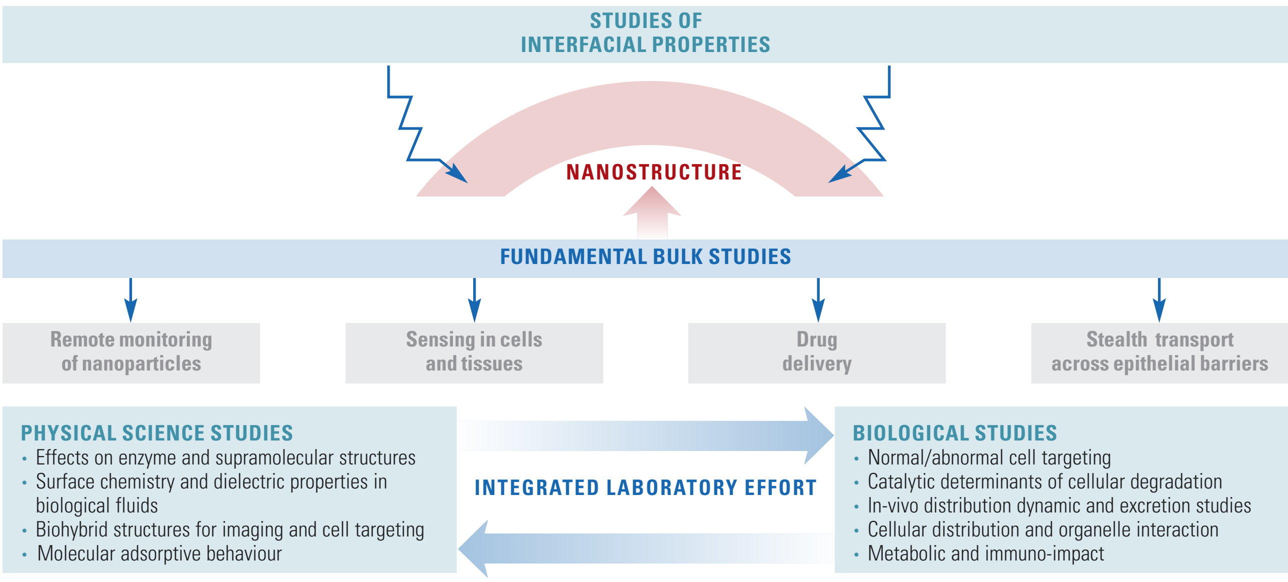


Fig. 11.5.15: Overview of nanomaterials in medicine.

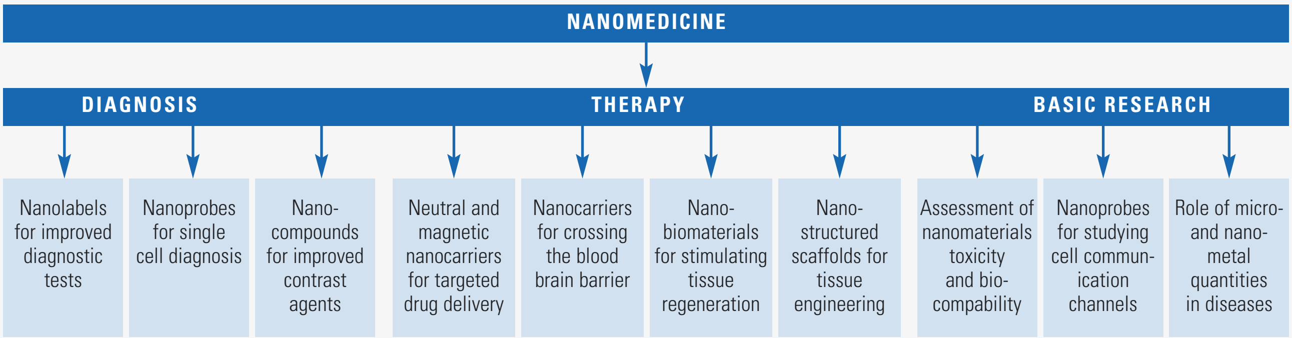


Fig. 11.5.16: Overview of the challenges for nanomedicine research.

techniques with advanced imaging and spectroscopy provide insight to the behaviour of single diseased cells and their micro-environment for the individual patient;

- Multifunctional contrast agents for medical imaging: New compounds directly responsive to biological activities. Efforts should be made to produce new diagnostic molecular imaging agents, but the most challenging part of this is delivering these multifunctional compounds to well identified targets.

2. Therapy

- Targeted delivery systems will play the central role in future therapy. Nanocarried agents will allow a localised therapy which targets only the diseased cells, thereby increasing efficiency while reducing unwanted side effects;
- The blood brain barrier usually prohibits brain uptake of larger molecules, which excludes many potential drugs for neurodegenerative or psychiatric conditions and in brain tumours. Nanocarriers with special surface properties may offer new and efficient options to carry a therapeutic payload through the blood brain barrier to deliver multiple therapeutic agents at high local concentrations directly to the target;
- Magnetic liposomes and binary shell poly-ferrofluids can be charged with high concentration of drug atoms and can be injected intra-arterially and concentrated at the area of interest by magnetic gradients. Optimisation of the stability and biocompatibility of the compounds is to be strongly developed;
- Pluripotent stem cells and nanobiomaterials will be essential components of multi-functional implants which can react to the surrounding micro-environment and facilitate site-specific, endogenous tissue regeneration to be used to repair traumatised, degenerated or infarcted organs;
- Tissue engineering encompasses the use of cells and their molecules in artificial constructs that compensate for lost or impaired body functions. It is based upon scaffold-guided tissue regeneration and involves the seeding of nanoporous, biodegradable scaffolds with donor cells, which differentiate and mimic naturally occurring tissues. Potential clinical applications of tissue engineered constructs include engineering of skin, cartilage and bone for autologous implantation.

3. Basic research on cells and tissues

- The same unique physical and chemical properties that make nanomaterials so attractive may be associated with their potentially toxic effects on cells and tissues. The existing and emerging uses of nanoscale materials have given rise to growing concerns about their unintentional health and environmental impacts: i.e. the metal oxide-based nanoparticles (TiO_2, ZnO, Fe_3O_4, Al_2O_3, and Cr_2O_3) and quantum dots have a core made up of relatively toxic metals (Cd, Se, etc);
- The indirect communication between cells, also indicated with "bystander" effect, needs investigation as a possible way to understand the individual response to radiotherapy during a tumour treatment. Nanobeams able to target individual organs of a cell are ideal tools for studying communication and cell mechanism trigger effects. Those studies should be combined with theoretical modelling of DNA damage for a detailed understanding of the cellular response to radiation;
- Metal ions play a multifold role in numerous cellular regulatory processes and can promote responses that range from deficiency to toxicity. Metals are known to play a major role in carcinogenesis and in the development of neurodegenerative diseases (like Alzheimer's). Static and kinetic studies of metal accumulation are critical for a better understanding of diseases' aetiology and to formulate new therapy strategies.

Impact of synchrotron radiation and neutron sources (Fig. 11.5.17)

- X-ray fluorescence nanoprobes appear to be a unique analytical technique with the adequate spatial resolution to examine intact hydrated samples at the nanometre scale. This technique is capable of both imaging, and chemical determination and speciation of metals. High-resolution/high detection efficiency/spectroscopy will allow to access to the three key parameters: spatial distribution (localisation), concentration (dose) and chemical state (coordination);
- Imaging will play an increasing role in understanding the characteristics of nanomaterials, since it complements bulk measurement methods such as scattering and spectroscopy by providing location specific information in heterogeneous systems;
- Ultrastructural x-ray imaging methods using synchrotron nanotomography coupled to elemental and speciation nanoanalysis will

be particularly suited to studies on the interaction of nanomaterials with biological structures;

- High resolution in-vitro and in-vivo imaging are needed for the follow up of a large number of nanoscale treatments. Those include accessing of kinetics of contrast agents in animal models, crossing of the blood brain barrier of nanocarriers, localising nanostructures in the tissues, studying the migration and differentiation of stem cells in samples. Ideal in-vivo techniques are K-edge and phase contrast imaging techniques available at synchrotron radiation sources;
- Patient treatment and related preclinical research should be developed for Stereotactic Synchrotron Radiation Therapy-SSRT and Boron (Gadolinium) Neutron Therapies-B(Gd)NCT, which are respectively synchrotron radiation and neutron specific techniques, targeting aggressive brain tumours, previously charged by highly concentrated nanotransported drugs;
- Focusing x-ray beams to nanometric scale calls for the development of long beam lines. Sample preparation and characterisation facilities in close proximity to the experimental stations are crucial;
- Sample management: develop handling methodology for fragile or nanoscale samples and to minimise sample radiation damage;
- In the detection of trace elements or in the structural analysis of nanomaterials, an increase of flux and brilliance of the source are strongly needed in conjunction with improved detectors;
- Nanoimaging and nanoanalysis beam lines with their associated specific stringent infrastructure issues: mechanical and thermal stability and coherence preserving, nanofocusing x-ray optics;
- High sensitivity and high speed x-ray detectors;
- Software to simulate nanofocus beam lines as well as fast data reduction and storage of copious amounts of data.

Needs for developments at large-scale facilities

- Prepare for nanofocusing optics, nanopositioning instrumentation, and high stability setups for x-ray nanoimaging and nanofluorescence;
- Develop dedicated biological and biomedical beam lines and facilities for in-vivo analysis of nanomaterials;
- Set-up large scale networks for analysis and modelling of biological systems (DNA, cells) and their interaction with radiation;
- Develop the complementarity and the integration of synchrotron radiation x-ray microscopy with other components of the microscopy community;
- Promote synergy between European laboratories (EMBL, ESRF, ILL etc.) and national synchrotron facilities to develop common strategies and infrastructures for nanomedicine.

Key elements of synchrotron radiation and neutron sources in the European Nanomedicine Centre

- High resolution structural analysis of nanodrugs in cells and tissues.
- In-vivo kinetics of distribution and biointeraction of nanodrugs in living models.
- Clinical application of synchrotron radiation and neutron therapies.
- On site cell and tissue culture and in-vivo biological facilities for preparation and analysis of cells, tissues and living samples.
- Availability of additional analytical facilities for protein and lipid biochemistry, drug analysis.

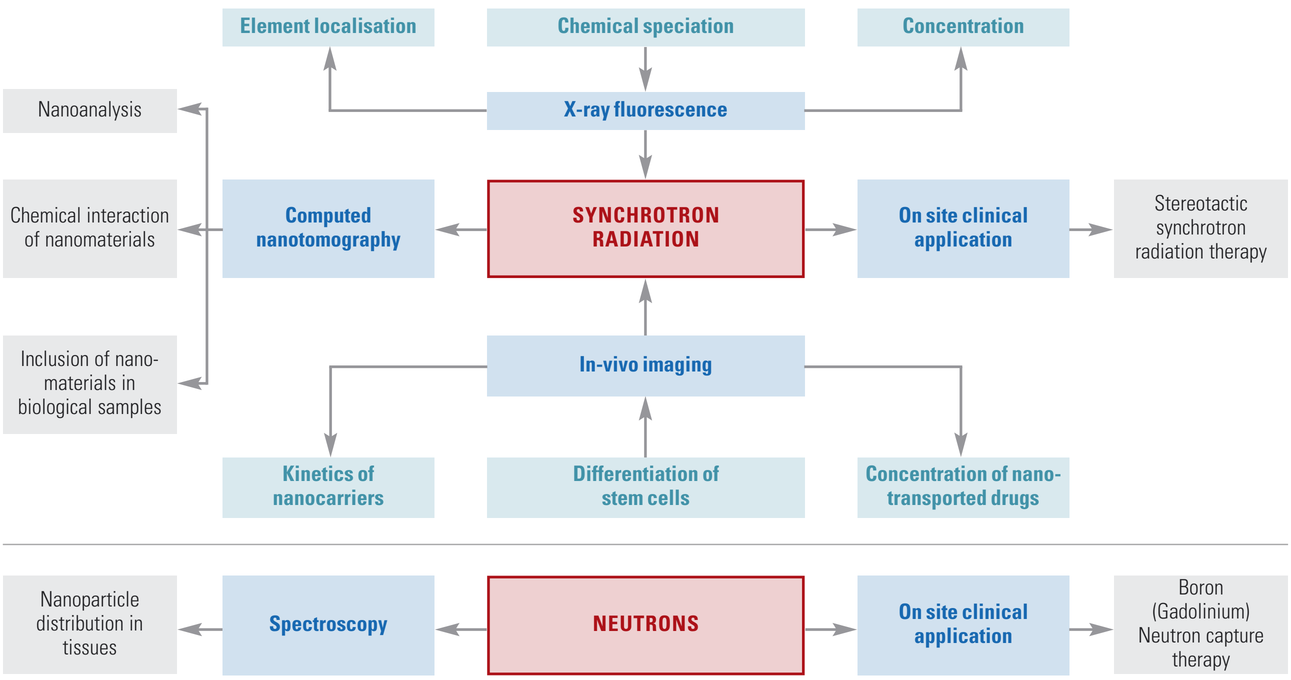


Fig. 11.5.17: Model for a European nanomedicine research programme and centre: "Role of synchrotron radiation and neutrons".

- **Dentistry**
- Self-assembling peptide scaffolds need to be designed which will interact with the mineral component for repair of tooth enamel and dentine;
- Injectable nanospheres and nanoparticles should be advanced for antibiotic delivery and periodontal disinfection;
- Targeted nanosensors for diagnosis of tooth related, oral and systemic diseases;
- Existing scaffolds for periodontal bone regeneration need to be improved with nanoscale grain sizes and hence provide superior mechanical properties, that can be used in load-bearing locations;
- Dental implants with nanotextured and coated biomimetic, antimicrobial surfaces need to be engineered for targeted cell differentiation and regeneration of periodontal tissue;
- Nanocomposite filling materials require to be investigated with improved aesthetics, longevity and mechanical properties.

Synchrotron radiation and neutron facilities are needed for:
- Neutron reflectometry to study the interfaces in implant materials;
- H_2O /D_2O contrast variation neutron tomography to assess the permeability of dentine after various treatment modalities;
- X-ray nanoscale probing of texture and composition in teeth sections using x-ray diffraction and nanofluorescence;
- X-ray tomography and x-ray microdiffraction of bone and soft tissue scaffolds and tissue-engineered hard tissue.

- **Pharmaceuticals**
- Nanoconstructs need to be developed as drug transport systems for tissue targeting;
- Multifunction nanoparticle capabilities need to be combined with drugs to enable in-vivo monitoring and directed transport of drug agents;
- Tailored release dynamics for drugs need to be engineered by manipulating surface and bulk properties of drug nanoconstructs;
- Drug transfer through cell compartments needs to be evaluated and optimised for effective therapeutics with reduced adverse effects.

Synchrotron radiation and neutron facilities are needed for:
- Neutron reflectometry to study drug properties at surfaces;
- SAXS/WAXS to follow molecular release behaviour at nanostructures;
- Neutron reflectometry to assess lipid films and nanoparticle/nanodrug interactions assessed at microscopic level;
- Time resolved x-ray and neutron probes for the kinetics related to transport of nano-pharmaceuticals in biological matrices;
- Rapid release kinetics of nanostructured drug carrier at cell and mucosal (e.g. nasal, intestinal) barriers;
- In-situ analysis of macromolecular and nanoscale drug carrier transport in intestinal tissue;
- In-situ analysis techniques for monitoring of nanoscale drug complexes in biological tissues and bridging of macroscale (ultrafast) kinetic data with traditional pharmacokinetics.

- **Healthcare/cosmetics/ointments**

  Hybrid systems for controlled skin interactions need to be engineered to provide for more specific effects:
- Controlled release materials for delivery of chemical modifiers and protective agents need to be optimised;
- Development of cosmoceuticals with nanosized particles for drug delivery;
- Stealth structures for dermal drug delivery and immunisation, including DNA vaccines in order to create non-injection routes to delivery;
- Self-organised structures for controlled skin coverage;
- Improved solar and environment protection nanocosmetics;
- Nanophotonic properties in cosmetics for better aesthetic properties;
- Controlled optical absorption materials to be refined and optimized;
- Light and environmentally reactive nanomaterials.

Synchrotron radiation and neutron facilities needs are:
- X-ray and neutron reflectometry for fast kinetics of reactive species generation (e.g. free radicals) under controlled photon exposure;
- Surface interactions between macro-/microsolutes and microbial flora in the skin;
- Surface molecular conformational change at functionalised nanoparticles for transcutaneous transfer of drugs.

- **Agriculture**
- Development of smart delivery nanosystems for prevention, improved diagnostics and treatment;
- Tailored syntheses of nanostructured bio-catalysts;
- Development of simple and smart delivery nanosystems for controlling and targeting bio-pesticides and nutrients;
- Preparation of nanobased filters and catalysts to reduce pollution;
- Development of autonomous nanosensors for real-time monitoring;
- Increase the efficiency of nanostructured biodegradable materials.

Synchrotron radiation and neutron facilities should provide:
- SAXS/WAWS to monitor nanoobject formation and evolution;
- Microtomography to investigate the nanomorphology of raw and transformed agri-materials;
- X-ray, UV and IR microanalysis and microimaging to investigate the chemical and structural behaviour of tissues when submitted to environmental changes or during industrial processes;
- Protein and polysaccharide folding dynamics at surfaces;
- H_2O dynamics and exchange across surface bound, gel-like and free water for modified surfaces and their correlation with protein denaturation.

- **Food** (Fig. 11.5.18)
- Understanding separation, emulsification and filtration technology, i.e. impact of changing ingredients during processing, texture modification with new manufacturing processes;

- Understanding the changes that occur to the ingredients during processing – real-time experiments is vital here. This will require the construction of novel cells to sit in the beam to permit accurate mimicking of processing conditions;
- Achieve multi-phase interactions in food-stuffs as nanocomposites, correlation of architecture with texture and quality and the non-equilibrium behaviour;
- Develop intelligent packaging materials and encapsulated components for slow release of flavours – extended lifetime and nutriceuticals – quality monitoring;
- Develop better use of food waste – either for other products in the food chain, or for novel products such as adhesives, packaging;
- Assessment of the quality of raw animal and vegetable materials and natural products, particularly as new crops may come into play due to the impact of global warming;
- Understand the role of trace components in affecting microstructure and how their distribution affects their nutritional impact;
- Understand how fat, sugar and salt content can be reduced and fibre content be increased, to give acceptable food quality (texture and taste) for the consumer;
- Understand how all these above factors affect slow changes in structure during prolonged shelf-life;
- Devise novel routes to produce dry foods that can be reconstituted in-situ to minimise transportation of water, by understanding the moistened to dry interconversion of food and its effects on nanoarchitecture; Understand diffusion dependence of solutes through food products and dependence on nanoscale organisation;
- Explore the degradation of food during chewing and digestion, to understand the location and kinetics of the release of the molecules into the gut and hence the bloodstream;

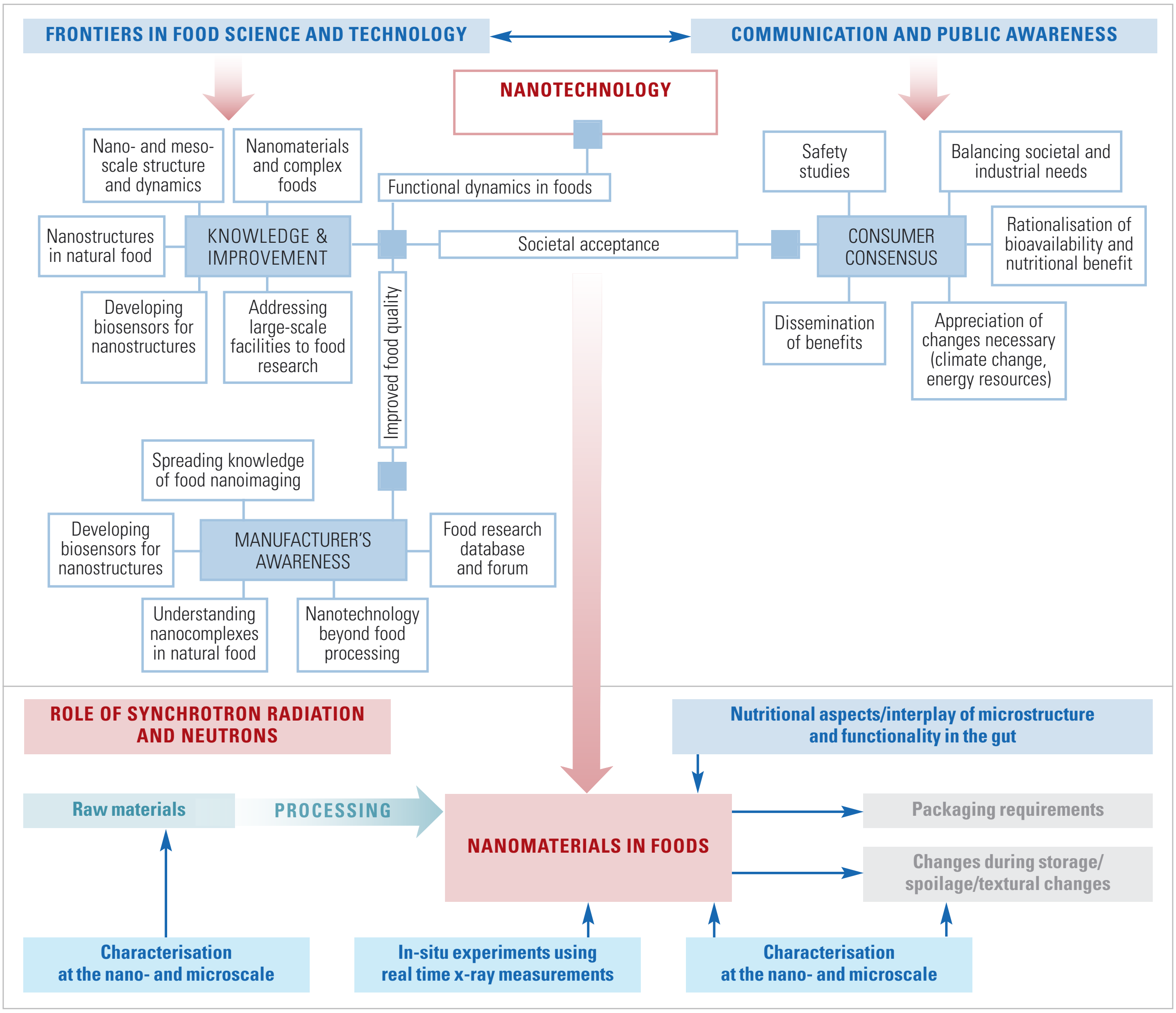


Fig. 11.5.18: Overview of the research needs on nanomaterials from a "knowledge and improvement" and a "consumer consensus" to define borderlines of advances in science and technology for food. Below, an overview of the characterisation on nanomaterials during the food cycle is shown.

- Advance new nanocomponents for nutrient and therapeutic component intestinal release and absorption;
- Develop tailored sensing and diagnostics with a chain approach for safety assessment.

Synchrotron radiation and neutron facilities should provide: (Fig 11.5.18).
- Micro- and nanoresolution 2-D and 3-D imaging and microanalytical techniques using IR, UV and X-photons;
- SANS/WAXS beam lines for investigating soft-condensed matter under various constraints and in various simulating life environments;
- SAXS/WAXS tracking of drug release from different components of nanocolloid and nanostructured drug carriers;
- Rapid kinetics of nanostructured drug carrier at cell and mucosal (nasal, intestinal) barriers;
- In-situ analysis of macromolecular and nanoscale drug carrier transport in interstitial tissue;
- In-situ analysis techniques for monitoring of nanoscale drug complexes in biological tissues and bridging of macroscale (ultrafast) kinetic data with traditional pharmacokinetics;
- Investigation of structure on molecular, nano- and mesoscales using wide- and small angle scattering and reflectometry facilities;
- Application of established concepts in soft materials and biomaterials science;
- Investigation of dynamics, kinetics and aging using bulk and surface spectroscopy over fifteen decades of dynamic ranges available at large-test facilities;
- Synergetic application of experimental techniques and advanced computational methods, including molecular dynamics simulations and quantum chemical calculations;
- Study of buried solid-liquid and solid-solid interfaces with x-ray and neutron imaging coupled with coarse-grained simulations;
- Interpretation of structured and dynamic results with insight derived from nanomechanical and nano- and micro-fluidic approaches.

- **Natural nanosystems**
- Modelling of hierarchical structures that mimic Mother Nature;
- Ability to monitor dimensions by designing specific natural macromolecules such as hybrid oligosaccharides or polysaccharides based block copolymers;
- New nanostructured biomaterials obtained from the self-assembly of natural molecules;
- Development of smart nanoparticles and surfaces decoration for drug delivery, improved diagnostics and treatments;
- Improve the host-guest biocompatibility for medical applications;
- Nanoparticles encapsulation for many application with "time-released" natural process;
- Increase the efficiency of nanostructured biodegradable materials;
- Mimics the nanostructured natural assemblies to build stimulable biomaterials;
- Nano-insect robots, nanoflying objects, nano-electromechanical systems, nanobiosensors, and flexible electrical displays using renewable raw materials;
- More environment-friendly and sustainable resources such as cellulose or cellulose-based materials;
- Design and fabricate new class of functional polysaccharide-based material having structures ordered down to the nanoscale level, for different applications including conducting thin films (flexible electronic devices) and microelectronic devices;
- Hybrid sugar-peptide and hybrid sugar-synthetic block copolymers;
- Self-assembling of hybrid block copolymers: nanoparticles and thin films and smart surfaces;
- Open new horizons and opportunities for block copolymer cellulose based thin film applications (flexible electronic nanodevices);
- To go to the lower possible limit in terms of size, spacing and high density for further applications and if possible below 15 nm such as for photonic application where quantum confinement becomes important.

Synchrotron radiation and neutron facilities are needed for the study of:
- Elastic and dynamic properties of single molecules, nanoparticles, surfaces or bulk materials;
- Nanostructural hierarchy;
- Time-resolved changes in the nanostructures;
- Rheological behavior under shear;
- Combined scattering and rheo-optical behaviour;
- Block copolysaccharide self-assemblies, nanoparticles and organised thin films;
- Dynamics at nanosurfaces;
- Deuterium labelling of natural molecules and neutron scattering investigations for structure (SANS & USANS) and dynamical properties (spin-echo);
- Decoration of nanoparticles or thin film with natural molecules;
- Smart surfaces with precisely nanostructured density of natural functionalities (oligosaccharides or polysaccharides).

Conclusion

Synchrotron radiation and neutron facilities are exceptionally matched to the challenge of nanotechnology: they offer the opportunity for precise, non-invasive metrology at ultra-short length scales and can couple this with information dense characterisation of interfaces and surfaces. The latter is of particular value, as the relative dominance of the interface versus the bulk of nanostructures drives much of their function in biology.

Whilst synchrotron radiation and neutron facilities constitute a major resource, they are also remarkably versatile in both the nanomaterials they are able to characterise by novel in-situ and in-vivo diffraction and imaging techniques with unprecedented capabilities to underpin advances in the research and development of bio-nanosystems, from a fundamental understanding of static and dynamic phenomena to the precision control of manufactured products in areas as diverse as medicine, pharmaceuticals, agriculture, health care, foodstuff and biomaterials. They will provide breakthroughs in:

- Dynamic imaging of natural and artificial nano-objects in cells, tissues and nanostructured biomaterials;
- Ultralow contaminant detection for toxicology analysis associated with nanostructures;
- Real -time monitoring of self assembly of nano-objects;
- Time-resolved follow-up of structural and chemical changes during the early stages of formation of nano-objects or when interacting with substrates;
- Tracking of multifactorial biological interactions of nanodrug delivery vehicles, and at multiple time scales to help develop a better pharmacdynamic understanding;
- Manipulation of the nanoparticle ageing process at the subcellular level and optimisation of recycling of nanoparticles;
- Advanced synergies with photoactivation and radiation linked therapies to give precision in tissue and cell level targeting.

GENNESYS will play a driving role in the development of bio-oriented nanotechnologies because large-scale facilities constitute a particularly favourable ground capable to match the technical demand from academic researchers as well as industrialists.

Strategy for a multidisciplinary European Research Programme and Research Centre

The research strategy should focus on the development of a collaboration of and the synergy between the various bio-nano-areas: nanomedicine, dentistry, pharmacy, health care, agriculture, food and natural nanosystems.

The European research programme should direct into new approaches for diagnostics, preosthetics and drug delivery systems. Focus should be placed on:

i) Planet benefits:
- New sources of bio-energy;
- Improved utilisation of land and resources;
- Product quality and preservation.

ii) Health benefits:
- Understanding of relevant toxicology;
- Development of nutricentials;
- Life quality;
- Worldwide protection.

In order to be successful in these ambitions, the use of synchrotron radiation and neutrons is vital, therefore these large-scale facilities need to have a suitable place in the development of a European nanobiosystems programme and institution. A model for the integrated nanomedicine, dentistry, pharmacy, health care, agriculture/food science programme and institute is schematically represented in Fig. 11.5.19.

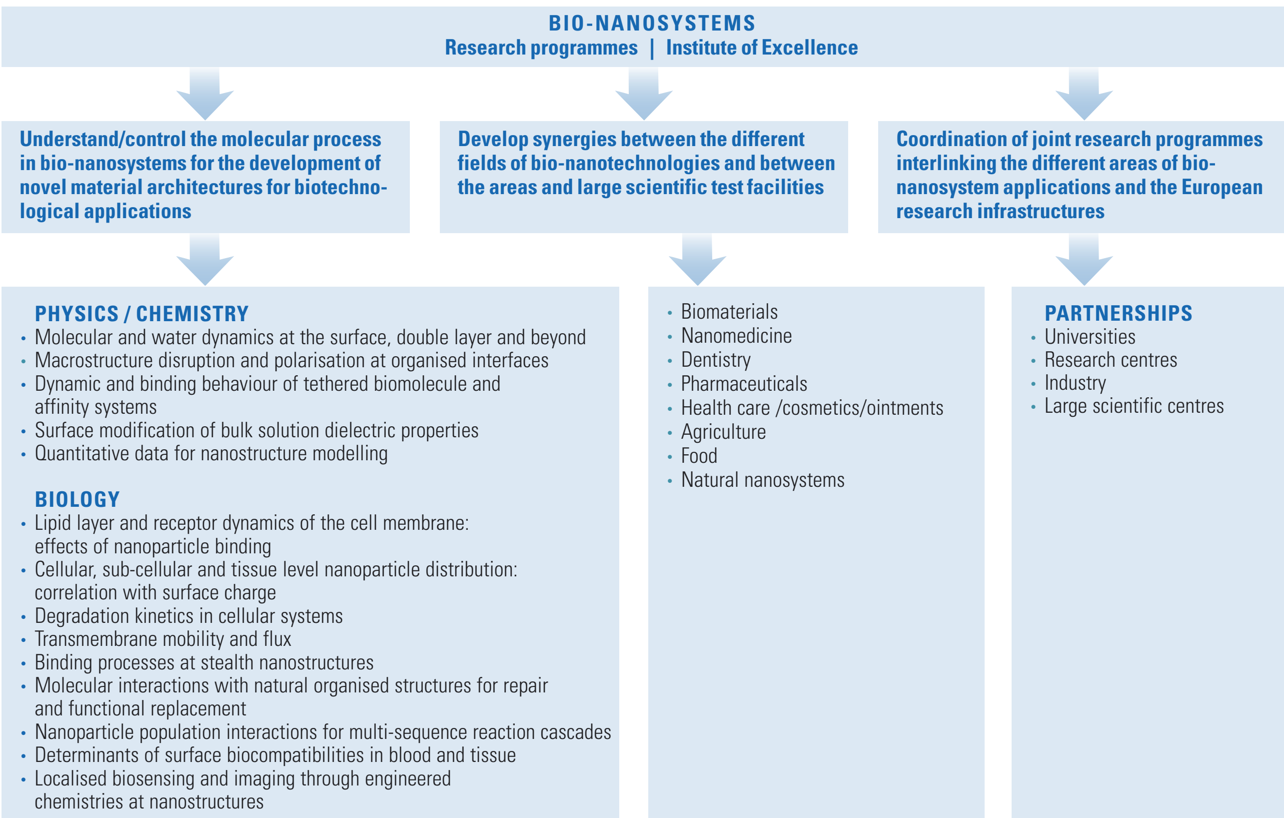


Fig. 11.5.19: Model for a European Bio-Nano-Interdisciplinary Strategy.

The execution of such an ambitious programme demands a long-term collaboration: excellence, free research, and could be best executed in the framework of a European Centre of Excellence. The principle lay-out of a European multi-disciplinary bio-nanosystems research centre is schematically represented in Fig. 11.5.20.

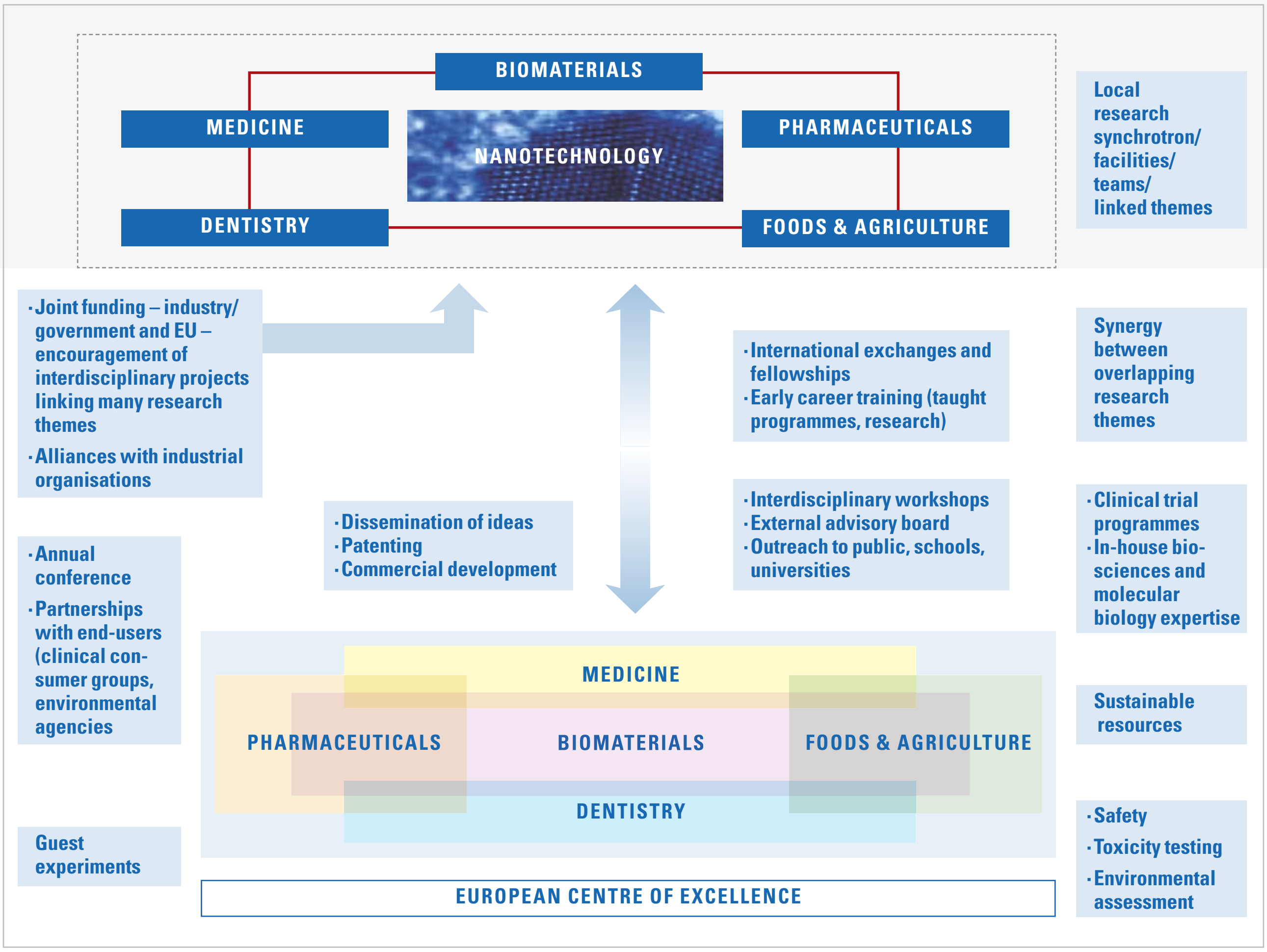


Fig. 11.5.20: Model for a European multi-disciplinary bio-nanosystems research centre.

11.5.4. CHEMICAL AND RELATED INDUSTRIES

Introduction

Nanomaterials are a key element in chemical-, oil- and petrochemical industry – both on the process side and on the chemical product side. In more than 90% of all the chemical products a heterogeneous catalyst is involved, mostly based on highly sophisticated nanomaterials. In future, the nanochemical products will attract much attention in polymer materials science, healthcare, sensor technology, biology, medical and health, energy including biomass and solar energy conversion, etc.

With the new challenges we are confronted in the field of energy conversion, bio-energy, environment, food and agriculture but also new consumer products, the future need for smart nanomaterials is more than obvious. These are preferentially not designed by trial and error but on the basis of a full understanding of the processes and functionality. Thus the key for new and tailored design of nanomaterials with defined properties is the rational design with defined catalytic, electrical, surface and optical properties. This requires extensive knowledge of the structure-property relationships, where synchrotron radiation and neutron sources will play a key role.

Research strategy

In order to meet the challenges in the field of energy, environment, food and new multifunctional products, major breakthroughs are required, that are:

- Ultrafast techniques to study processes in real-time on an atomic scale;
- Spatial information on an atomic scale' imaging on a nanoscale;
- Rational nanomaterial design on an industrial scale.

If characterisation studies can be obtained under realistic process conditions, this will help in a rational "bottom-up" design of materials with the desired catalytic, electrical, surface and optical properties; Fig. 11.5.22 gives an idea about the role of the synchrotron radiation and neutron research in this respect.

Guidelines for future European research directions

Breakthroughs for research and industrial innovation realising using synchrotron radiation and neutrons are summarised in Fig. 11.5.23.

Key areas for nanomaterials in chemical and related industries

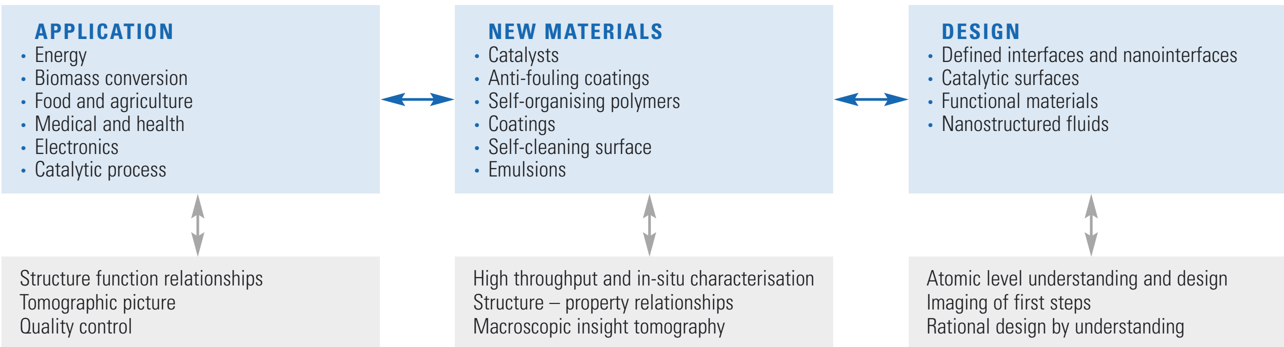


Fig. 11.5.21: Nanomaterial development and challenges from synchrotron radiation and neutrons.

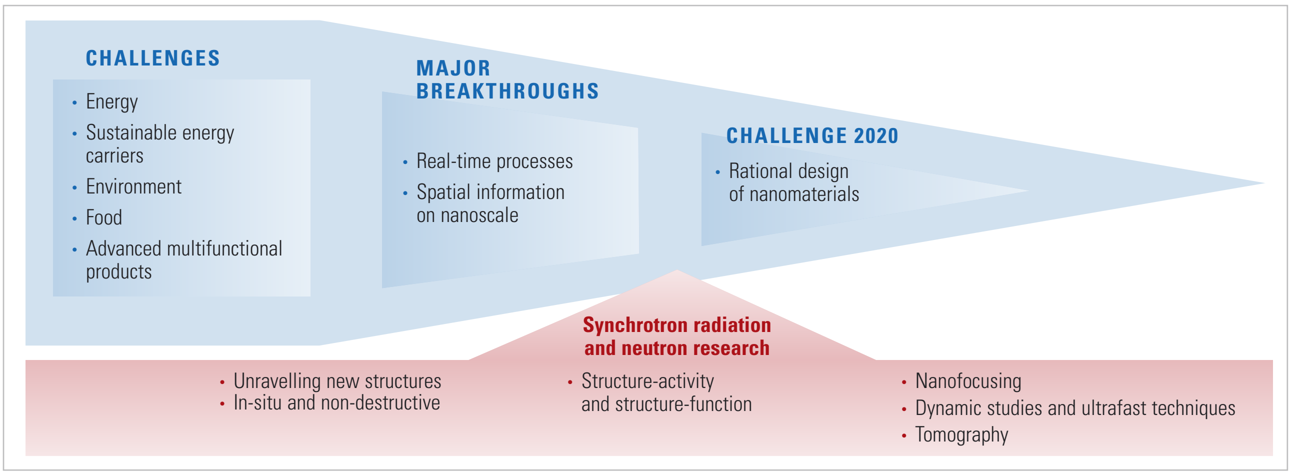


Fig. 11.5.22: Role of synchrotron radiation and neutrons in the chemical industry.

	NANOSTRUCTURED CATALYSTS	NANOMATERIALS IN THE CHEMICAL INDUSTRY	NANOSTRUCTURES IN THE PETROLEUM INDUSTRY
Challenges	Complex formation processes under demanding in-vivo conditions	Complex non-linear interplay between the phases in composite materials, formulations and bio-related structures	Complex interfaces in multicomponent systems (oil, water, rock)
	Complete quantitative multi-scale understanding of structure-property relationships		
Research for breakthrough	Describe the processes of catalyst formation under in-vivo conditions; Unravel catalytic processes in molecular detail	Full characterisation of the interfaces in multi-component systems of synthetic and biological origin	
	Combine experimental and computational efforts to cover all relevant length and time scales with emphasis on molecular and nanometric length scales		
Topics for SRN research	Time-resolved in-situ SRN experiments to unravel catalytic processes under realistic conditions	Characterisation of functional motives with emphasis on structural changes and interfacial substructures	Tomography of complex multiphase systems; selective marking of actives to elucidate mode-of-action mechanisms
	Complete mapping of structural and dynamic features covering the whole nanodomain (from 1 to 1000 nm) and all time scales (msec to days) by combining microscopic, spectroscopic and scattering techniques		
Industrial innovation	New and more efficient catalysts; new resource-saving processes	New materials and processes with benefits for environment, safety, health and well-being	Improved efficiency of established processes and exploitation of new approaches
	Rational and efficient design of structures, materials and processes		
Requests for SRN development	• In-situ characterisation of dynamic processes with suitable set-ups at the beam lines • Combination of various techniques (microscopic, spectroscopic, scattering) incl. non-SRN-methods at selected beam lines • Standardised sample mounting • Standardised data treatment, evaluation and visualisation		

Fig. 11.5.23: Highlights of nanomaterials in the chemical and related industries and the role of synchrotron radiation and neutrons.

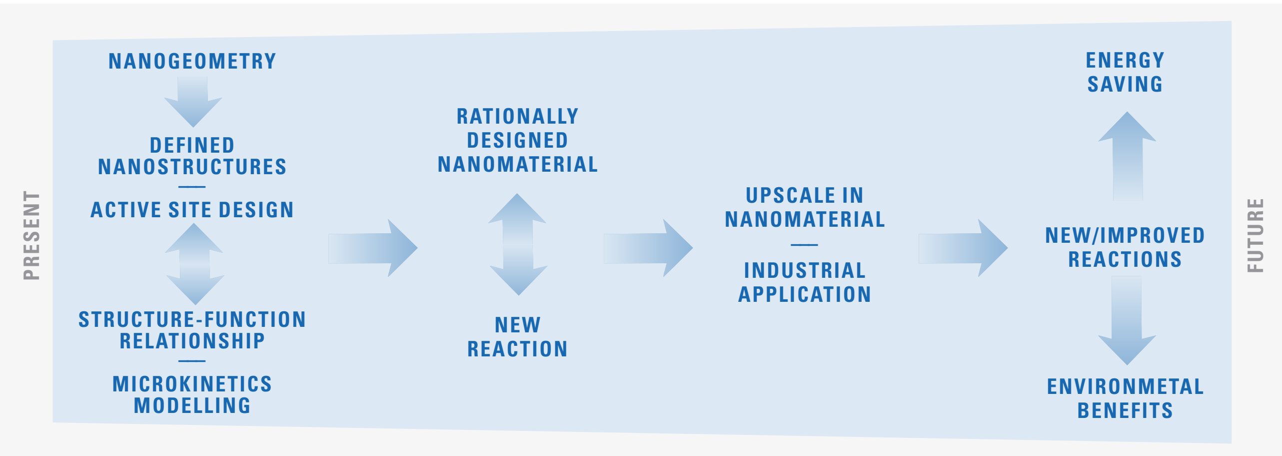


Fig. 11.5.24: Roadmap for nanocatalysis.

CATALYTIC NANOMATERIALS AND CATALYSIS: synchrotron radiation and neutron studies

Design and modelling of active sites, synthesis of nanostructured catalytic materials, operando characterisation of catalysts and catalytic reactions

Nano-imaging, 2-D and 3-D structures, structure of interfaces, valence/coordination states of active sites, stereochemistry of reactants and products, localisation and dynamics of reactant molecules, diffusion and permeation studies, structure of complex fluids, conformational analysis of supramolecular systems

ENERGY AND TRANSPORT

- Tailored catalysts for heavy oils and bitumen hydrotreatments
- Design of stable/recyclable nano-structured catalysts for gasification of biomass and production of synfuels
- Process intensification for energy saving, higher H_2 or hydrocarbon yields, and easier CO_2 capture.
- Theoretical modelling of active sites, kinetics modelling

- Tailored nanomaterials for improved H_2 storage
- Design of non-noble metal catalysts for fuel cells
- Semiconductors with high quantum yields and extended sensitivity to visible light

- Heavy fossil feedstocks processesing
- Energy efficient thermochemical processing of biomass/coal (Gasification, pyrolysis, deoxygenation, Fisher-Tropsch) to H_2 and hydrocarbons.

- Improved H_2 storage capacity (hydrides, solids)
- Intensification of fuel cells for mobile and stationary application
- Photocatalytic water splitting to hydrogen
- Conversion of water and CO_2 to methanol

CHEMISTRY AND PETROCHEMICALS

- Design of recyclable, nano-structured multifunctional catalysts
- Tailored catalyst resistant to poisoning for biomass processing
- Process intensification, coating of microreactors, monoliths, membranes

- Biomimetic catalysts for highly selective reactions at low temperatures

- Catalyst design and discovery via high throughput testing and combinatorial approach
- Immobilised organometallic catalysts resistant to leaching

- Synthesis of bulk/intermediate chemical...
- Conversion of biomass or recycled wastes (e.g. used polymers) to chemicals

- Activation of methane, selective oxidations, N-insertion

- Development of one pot, multi-step synthesis
- Selective synthesis of bioactive molecules
- Improvement of C-C coupling reactions
- Chiral catalysis

ENVIRONMENT

- Design and discovery of improved photocatalysts (quantum yield, extension of sensitivity to visible light)
- Nanomaterials for filtering of nanoparticles
- Tailoring of non-noble metal catalysts for oxidation or reduction reactions

- Catalyst resistant to deactivation (poisoning, leaching, attrition)

- Nanolayer coating of structured catalytic reactors (microreactor, monolith, membrane)
- Design of highly selective nano-structured porous membranes for gas separation (CO_2)

Air treatment
- Particulate removal from mobile and stationary sources
- NOx, VOC abatement
- Indoor detoxification (noxious bacterial agents)

Water treatment
- Removal/recovery of heavy metals
- Total oxidation of organic wastes (drinking water, waste water)

Greenhouse gas reduction
- Separation and capture of CO_2,
- CO_2 as building block for chemical synthesis
- Effects of aerosols on atmospheric chemistry

NANOBIOLOGY AND MEDICINE

- Conformational studies of enzymes
- Tailored nanomaterials for drug storage and delivery
- Design of supramolecular organic/inorganic catalytic systems
- Nanostructures for supporting enzymes

- Bio-/photo dissociation of water to hydrogen
- Bio-desulfuration
- Improved enzyme activity for biomass and waste fermentations to biogas
- Enzyme for chiral synthesis, food processing
- Bioactive molecule design and drug delivery

Fig. 11.5.25: Overview of nanocatalyst materials in multiple industries.

Catalysis in the chemical industry (Fig. 11.5.24)

- Key challenges are in the field of energy and hydrogen production from renewables, fine chemicals including chirality, selective oxidation, fuel cells and environmental catalysis (air and water treatment);
- Aim is the atom by atom design and manufacturing of catalysts with defined active sites;
- Important basis for this research is the identification of the active sites;
- Establishment of structure-performance relationships;
- In-situ studies of chemical processes on the surface in a spatio-temporal manner;
- Understanding the dynamics of reactant molecules on catalyst surfaces and the diffusion of reactants and products in catalyst pores and nanostructured reactors;
- Input to theoretical studies predicting the best nanostructures for a desired chemical reaction.

Catalysis in a multi-industrial environment

In future, nanocatalyst materials will play a vital role in the innovation in many industries. Fig. 11.5.25 summarises the potential nanomaterials developments, the research needs and the roles of synchrotron radiation and neutrons (see also Fig. 11.5.26).

New materials for coatings, smart packing materials and self-cleaning surfaces

- Key challenges are the development of new functional coatings with special optical properties, surface properties and nanostructures;
- Rational design of advances materials and composites;
- Establishment of structure-property functions that gives a fundamental understanding of the surface properties, interfaces and physical properties;
- Bottom-up design of new materials;
- Controlled growth, surface grafting and surface modification;
- Dynamics of the growth process.

Nanomaterials in the oil and petroleum industry (Fig. 11.5.28)

Many practical problems which are currently present in the petroleum industry are better controlled employing nanomaterials including nanoscale self-assembling soft matter materials. Problems range from the upstream oil production in oil wells, the transport of oil from well to storage and refineries, to the downstream refining process itself and the later use of oil products in combustion engines. A rational design requires a complete understanding of the hierarchical multi-scale nature of functioning nanomaterials over large ranges of distance and time. Instrumentation for neutron and x-ray diffraction stud-

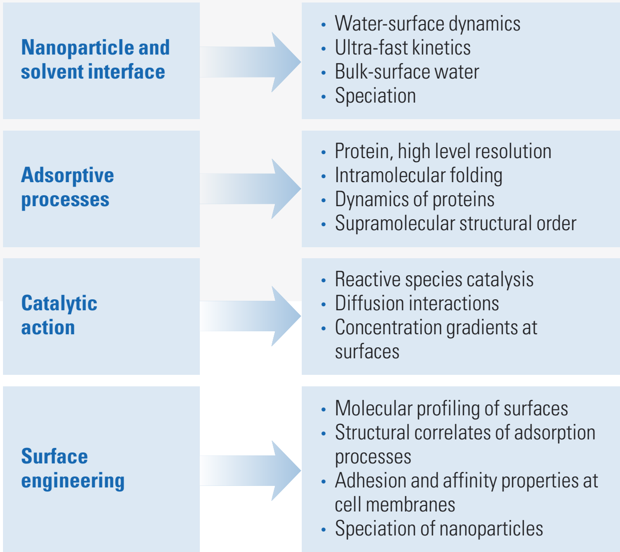


Fig. 11.5.26: Value added benefits of synchrotron and neutron sources in the chemical industry.

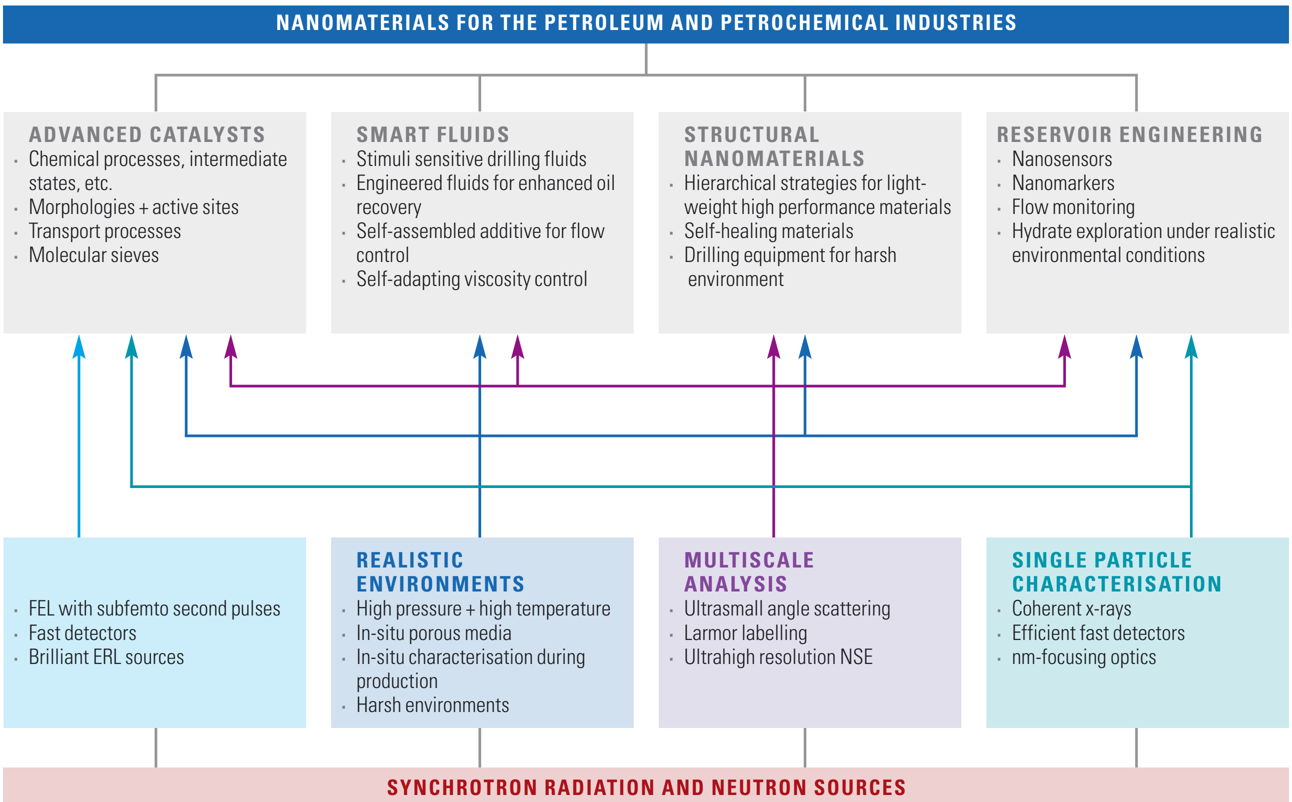


Fig. 11.5.27: European research programme on nanomaterials for the petroleum and petrochemical industries.

ies will have to cope with time and length scales ranging over many orders of magnitude. For example from attoseconds to monitor the functioning of a catalyst, up to macroscopic times relevant for flow properties of smart fluids and length scales from small aggregates of atoms in catalysts, to micrometre sizes significant for hierarchical assemblies. For the next decade and beyond, neutron and synchrotron scattering techniques will be essential for development in the following key areas:

- **Advanced catalysts:**
  - Real-time observation of chemical processes in the attosecond and femtosecond regime;
  - Characterisation of the nanostructured morphology and active sites;
  - Transport processes, molecular sieves to separate products;
  - Development of nanocatalysts for on-site field use.
- **Smart fluids:**
  - Tailoring of stimuli sensitive drilling fluids based on polymers, nanoparticles and surfactants for faster drilling and reduced wear;
  - Design of fluids with engineered amphiphilicity to control water, surfactant and oil flow for enhanced oil recovery;
  - Responsive materials e.g. shear induced gels to block fractures;
  - Development of nanostructured self-assembling additives for flow and crystallisation control.
- **Structural nanomaterials:**
  - Light-weight high performance materials based on engineered nanoparticles and hierarchical strategies;
  - Self-healing polymer nanocomposites for drilling under extreme conditions;
  - Nanocrystalline substances for durable drilling equipment.
- **Exploration and engineering of reservoir:**
  - Nanosensors for probing properties deep in the reservoir;
  - Nanoparticles as markers for improved sizing and characterisation of the reservoir;
  - Nanoparticles for fluid flow monitoring and fluid type recognition;
  - Exploration of hydrate properties under harsh environments.

In order to achieve maximum impact, it is suggested to implement nanoscience facilities at the sites of the best large-scale x-ray and neutron facilities in Europe. These facilities should follow an integrated approach featuring nanosciences, nanofabrication and characterisation, thereby each focusing on different fields in nanoscience. Nevertheless, each should incorporate aspects of the entire nanoscience spectrum, in order to exploit synergies between the different nanoscience branches. Fig. 11.5.27 presents the organisation of a European research programme on nanomaterials for the petroleum industry, displaying the research needs on neutron and synchrotron facilities.

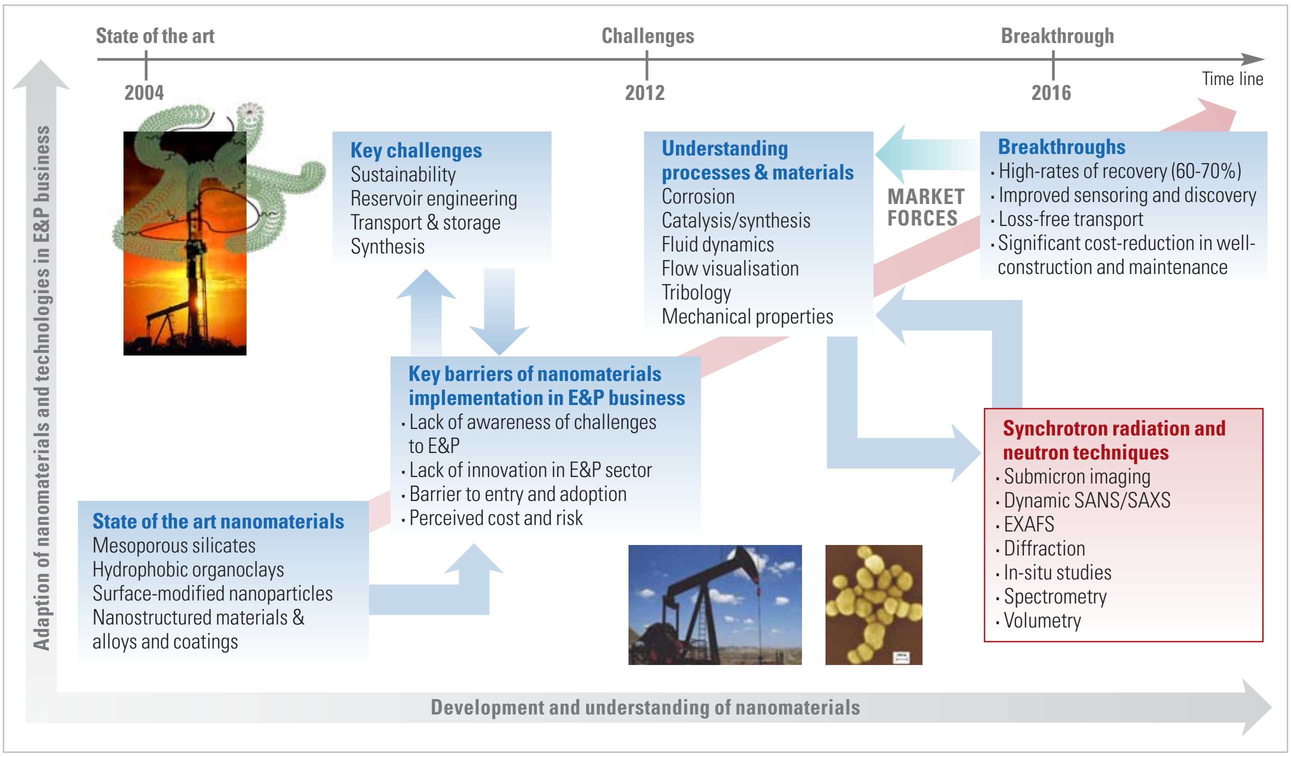


Fig. 11.5.28: Roadmap for nanomaterials in the oil- and petrochemical industry.

11.5.5. NUCLEAR TECHNOLOGY

The construction of modern fission and fusion reactors demands high performance structural and functional materials in order to assure reliable operation under extreme mechanical stresses at high temperature, in corrosive environments and under intense radiation exposure. These materials are presently not available although there have been continuous developments in the last few decades; a plateau has been reached and incremental improvements will be ineffective. New ideas and innovations in technology are needed and nanomaterials and nanotechnology offer challenges to realise breakthroughs (see Fig. 11.5.29).

Due to the complex nature of nanomaterials, a more fundamental approach in research is required in order to prepare tailored nanomaterials and to predict their lifetime in simulating nuclear environments. This opportunity can only be faced with the help of powerful analytical techniques like synchrotron radiation and neutron sources.

Fig. 11.5.29: Vision on future reactor technology and nanomaterials research and development.

Research challenges and the role of synchrotron radiation and neutrons

Highlights for research could be summarised as follows:

- To develop guidelines/models for the preparation of tailored nanomaterials: nanoparticles and fibres, ODS-NDS-CDS dispersion strengthened metallic materials and nanostructured ceramics- and composites;
- To study the creep, low cycle fatigue and crack propagation, over multiple length- and timescales, in simulating nuclear environments; for reliability and lifetime prediction purposes;
- To investigate the radiation damage processes of nanostructured materials stemming from new fission and fusion reactors;
- To study internal stresses under operational condition, non-destructively, via SANS;
- To measure the hydrogen isotope deposition patterns in 3-D fusion reactor component structures: neutron tomography;
- To investigate processes taking place at nanomaterial surfaces during plasma-surface interaction: neutron reflectometry;
- To measure the formation of chemical phases and the local atomic structure: in-situ: surfaces, interfaces and grain boundaries: high resolution EXAFS and NEXAFS techniques;
- To study the formation of brittle phases under fusion specific conditions: high intensity diffraction techniques;
- To quantify defects in materials at atomistic, nanoscopic and microscopic level: PALS (Positron annihilation lifetime spectroscopy) by using intense neutron sources for the generation of intense positron beams;
- To determine the chemical and structural environment of elements at low concentrations;
- To define the boundary conditions for reliable operation of structural nanomaterials;
- To define the criteria/parameters for optimum nanomaterial manufacturing routes.

The development of these new materials and their reliable behaviour in service will require testing devices which allow exploration at the nanoscale. In this context, synchrotron radiation and neutrons are of vital importance for the future research on nanomaterials and this to the welfare of the next generation's fusion and fission nuclear reactors.

Conclusion

Nanomaterials science and technology are necessary for the development of the new generation nuclear fission and fusion reactors. The inventions of these new nanomaterials will require great scientific potential in personnel and most advanced analytical measuring facilities; synchrotron radiation and neutrons will have to play a key role in these innovations especially for measuring "complex phenomena" in-situ.

11.5.6. ENERGY TECHNOLOGY

All energy foresight scenario's developed by different institutions arrive at the same conclusion that, for at least the next two decades, global energy consumption will increase continuously. This must be considered against a background of the need to assure security of supply, with dwindling natural resources, an ageing fleet of generation plants, and the need to protect our environment and global climate. In order to satisfy these competing needs, it is necessary to increase the efficiency of the use of conventional primary energies, decrease their carbon footprint, and to advance the development of renewable and nuclear energies. This social and political landscape, together with the mix of supply-side technologies, is shown in Fig. 11.5.30 and defines the landscape for any scientific and technological activity in the arena of energy technologies. The green triangle outlines the competing environmental economic and political drivers which inform the regulatory framework in which the energy markets must operate. These in turn will determine the mix of energy technologies shown in the red triangle. It is not in doubt that, across Europe, all these technologies will be needed to meet the demands outlined above, what is more questionable is the balance, i.e. where in the red triangle the final mix will sit. This scenario, and similar scenarios, are global, and thus represent a need for change in the energy supply industry on an unprecedented scale. This change will be extremely challenging to implement, but it also offers an enormous commercial opportunity for European industry to compete in this market and hence will contribute to continuing wealth creation in Europe.

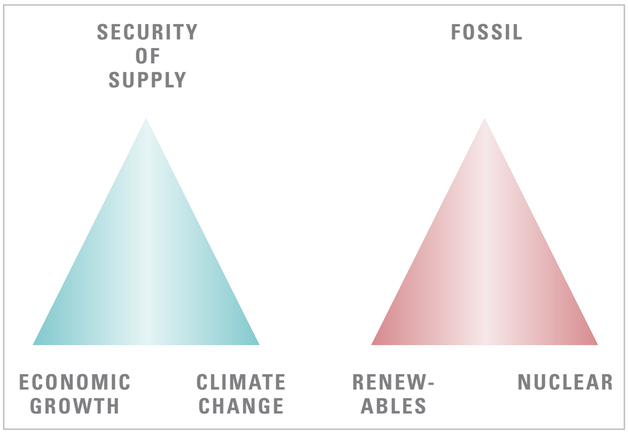


Fig. 11.5.30: The landscape for energy technologies.

Energy targets and challenges for research and development

The constraints described above provide a very strong technological pull on the development of energy technologies, and to meet this global agenda of carbon reduction and security of supply, an aggressive programme of technological and scientific development is necessary in order to achieve the necessary balanced energy portfolio. Some high-level goals of energy technology development can be summarised as follows:

- Increased efficiency of conversion;
- Reduction of cost;
- Higher performance in harsh environments;
- Plant lifetime extension;
- Reduce emissions;
- Reduction of development timescales;
- Demand reduction by increased efficiency of use.

In order to achieve these high level goals and to finally realise novel, efficient environmentally-friendly energy technologies, breakthroughs are needed in the underpinning discipline of materials science and engineering, spanning the whole range of materials types, from semiconductors and polymers to metals and ceramics. Achieving these breakthroughs will require an unprecedented and focused effort in materials, and here we will highlight the impetus that nanomaterials and nano-engineering can provide to this task, and how this critical materials development process can be accelerated by the deployment of state of the art facilities for the characterisation of materials at all length scales.

Materials research needs

The overall research needs on energy-related science and technology in which materials science at the nanoscale is expected to have a large impact are described with focus on:

- The discovery of novel materials;
- The fabrication and characterisation of nanomaterials and nanostructures.

Novel materials

For many of the device applications currently under development, suitable practical materials have yet to be discovered. There is thus the need for the continued synthesis of novel materials either by intuitive methods or by the more pragmatic methods of materials informatics and combinatorial methods. Time-resolved analyses involving very high brightness sources are invaluable in the determination of synthesis routes for novel materials. High throughput measurement and characterisation techniques will aid any combinatorial approaches. This continuing and urgent search for materials requires the ability to rapidly and accurately determine structure at the atomic scale and to probe local atomic environments. These structure determinations will complement efforts with atomic scale modelling to elucidate and hopefully predict materials properties from composition and crystal structure.

The fabrication and characterisation of nanomaterials and nanostructures

Although the search for new materials will always yield some spectacular results (an example is the discovery of high temperature superconductors), there are many areas of technology where materials performance is known to be very close to perceived theoretical limits. The much needed improvement of performance in many energy materials can be obtained by synthesising nanomaterials or fabricating nanostructures. These improvements in performance are not incremental. A startling topic is the recent discovery of colossal oxygen ion conductivity in thin multilayer heterostructures of nm-scale strontium titanate layers and yttria stabilised zirconia layers. Such paradigm shifting discoveries can revolutionise energy technologies, particularly in the application of functional materials.

This type of activity shifts the scientific focus from experimentation aimed at understanding bulk properties, to the study of materials that are dominated by the properties of their external and internal surfaces (both homogenous and heterogeneous), i.e. surfaces and interfaces. This shift of emphasis gives rise to the following analytical requirements;

- **Tailoring of nanomaterials** i.e. understanding and controlling the synthesis and mechanisms of growth of complex, natural or engineered, nanomaterials this requires the parallel develop-

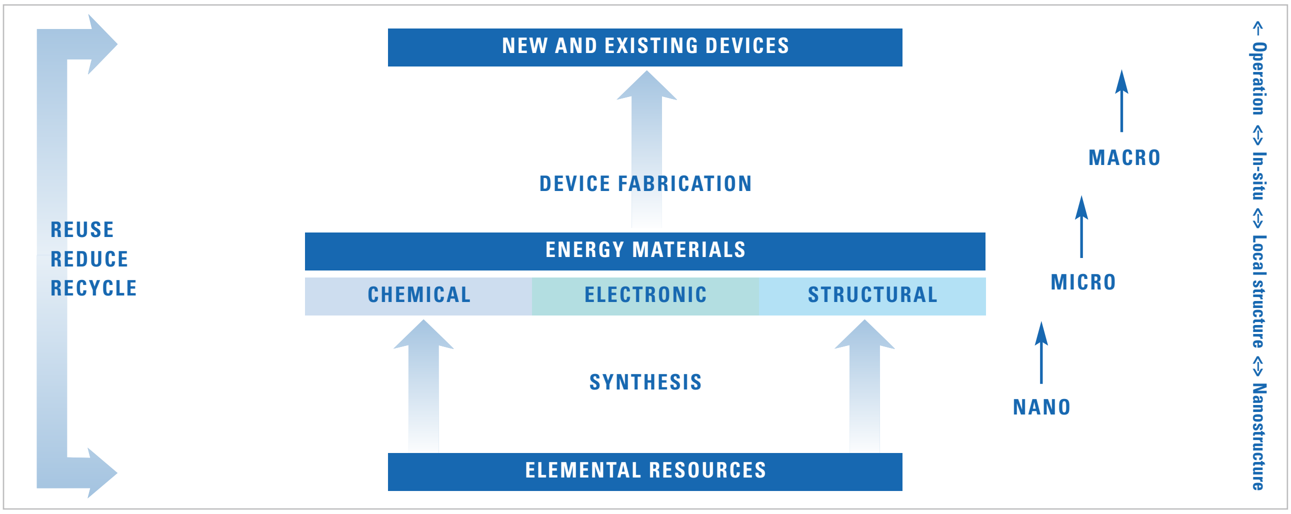


Fig. 11.5.31: The materials development cycle.

ment of experimental approaches, modelling & simulation tools, and of time-resolved in-situ diagnostics of processing techniques.

- **Exploring the new and novel properties of nanomaterials** will require characterisation facilities that combine sample manipulation capabilities with imaging, in-situ property measurements and studies of activity under operating conditions. In particular the chemical and structural characterisation of interfaces will be of prime importance.

- **Commercial application of nanomaterial**s this will need the large-scale production of high quality nanomaterials and rapid QA techniques.

The research challenge is to tailor the interface functionality at the nanoscale, in order to optimise transport: for electrons and ions in devices such as fuel cells and batteries; sensors and supercapacitors. In order to create the novel nanostructures, a spectrum of synthesis methods should be combined, ranging from lithography, wet chemistry methods, self-assembling growth of materials, to biological assembly.

A topic for which a scientific breakthrough is urgently required is the solid state storage of hydrogen. Despite intensive research efforts devoted to finding practical hydrogen storage, particularly for mobile applications, current materials do not meet the stringent performance targets. Nanomaterials and nanostructures offer the potential to fulfil this role.

In general terms, nanomaterials and nanostructures can tremendously enhance the performance of the whole range of energy materials and accelerate the materials development cycle shown in Fig. 11.5.31. To illustrate this possibility, three example areas of chemical, electronic and structural energy materials are described below, where the application of synchrotron and neutron radiation sources can make a critical contribution. A more detailed matrix of the applicability of these techniques in the areas discussed is given in Fig. 11.5.32 and Table 11.5.1.

Chemical and electrochemical energy materials

Chemical reactions obviously play an essential role in energy conversion, transportation, chemical manufacturing and environmental protection. This is especially true for energy production processes where a catalytic reaction takes place. Nanostructured materials provide an extraordinary opportunity to dramatically improve catalytic performance. The research challenge in nanoscience for catalysis is to tune the energy landscape of the nanostructured catalyst materials with the chemical reactants. The following reactions take place at the nanometre scale: the interaction of reactant gases with solid-state compounds in fuel cell electrodes, gas separation by membranes, catalytic reforming reactions of hydrocarbons. Improvement of the performances implies improved knowledge of the chemical reaction in question, and this requires new efficient and accurate methods for in-situ and characterisation under operating conditions.

The majority of methods to transform and store energy implement the inter-conversion of chemical species or the transport of energy in forms of ions. This is especially true when electrodes are considered (batteries, supercapacitors, fuel cells). Here, the transport of the active species through complex interconnected parts can be largely limited by the poor quality of interfaces. Transport can take place both across and along the interface and can either delay or enhance and can thus have profound effects upon device performance. Interfaces have to be regarded as complex nanostructured junctions of both similar and dissimilar materials that play a key role in the behaviour of nanomaterials and nanostructures.

Electronic energy materials

Electronic energy materials are materials that can perform the direct conversion of electronic energy into diverse forms such as heat, light and vice versa. These materials are used in devices such as photovoltaics, LED's thermoelectric generators and coolers, and rely upon the interactions that occur at interfaces and surfaces. An example is the photon absorption and intrinsic charge separation that takes place in photovoltaic cells. The research challenge is to tailor the interface functionality at the nanoscale, in order to optimise transport: for electrons, for electrons and phonons (thermoelectrics), photon collection (photovoltaics), for electron and hole recombination (lighting).

An example of where a breakthrough in materials could have a profound impact is the development of a high efficiency green LED for white light generation. No material exists at present to generate green light with a high efficiency, however such a material could lead to the widescale adoption of low voltage high efficiency lighting with a consequent major impact on the reduction of demand.

Structural energy materials

Many processes developed for the production, storage, and conversion of energy carriers hinge on the mechanical stability of structural components. Here, one could think of wind transformation, nuclear fission, nuclear fusion for conversion processes, and super-strong light-weight materials for transportation. The development of future technologies (nuclear fusion) will require new construction materials. Opportunities are offered for revolutionary advances through the discovery of new nanostructured materials and establishing new methods to fabricate them, including nanoscale self-assembly.

Studying the degradation of nanomaterials in simulated extreme operating environments (high temperatures, corrosive environments, mechanical stress) and after a long operating lifetime offers another great opportunity. The purpose of this research should be to predict the lifetime of the installation, or alternatively to discover processes that can operate at moderate conditions in order to eliminate barriers to developing new energy resources.

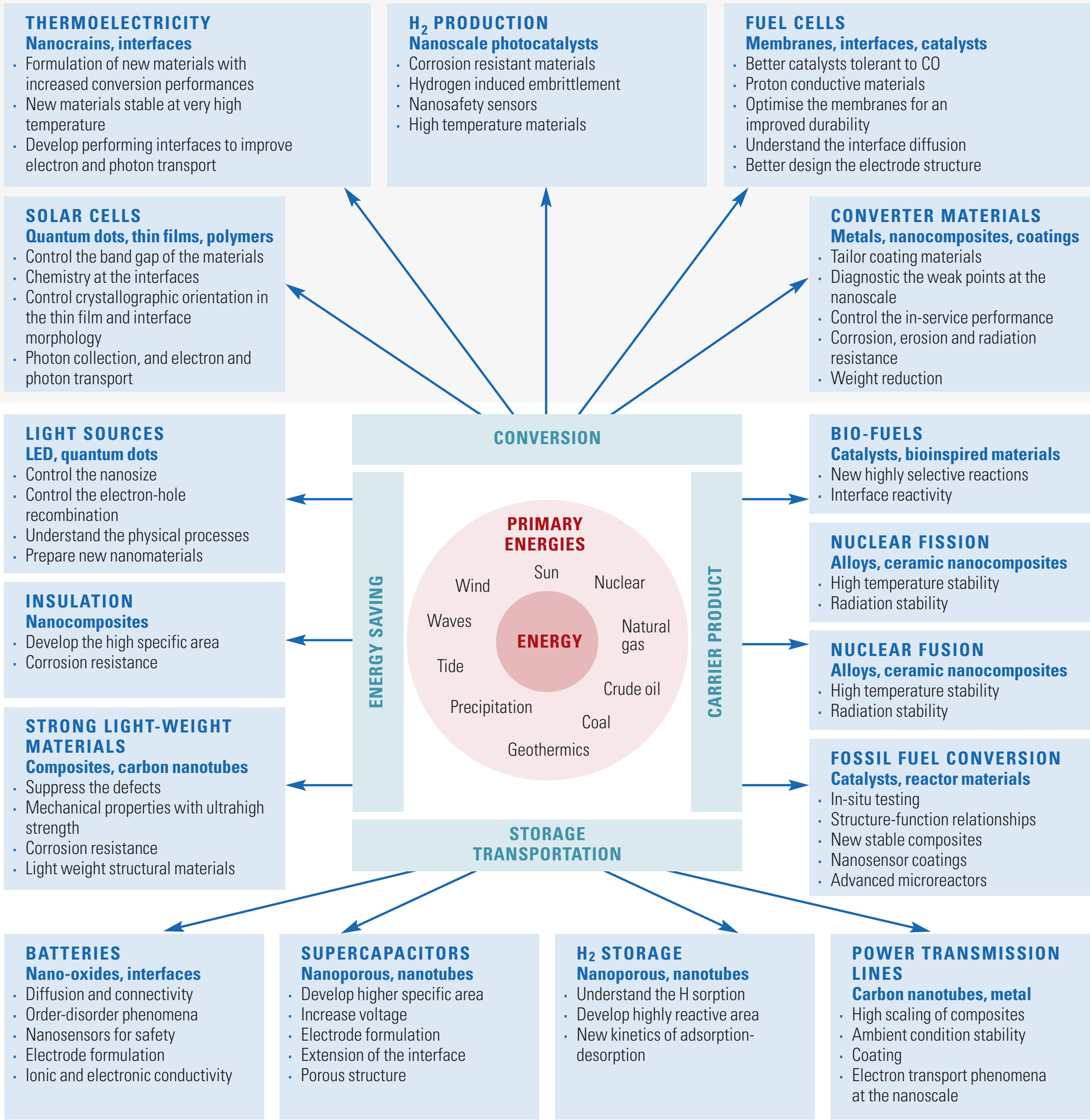


Fig. 11.5.32: Energy targets and challenges for research and development.

Role of synchrotron radiation and neutrons

In the different steps from the synthesis of new nanomaterials to their use in dedicated set-ups for the production of energy carriers, transformation of energy or efficient energy use, there remains the question of the structure of the material and the reactivity of the involved species. In order to unravel the processes governing the performances and durability, there is a need for advanced investigations which explore the true promise of novel nanomaterials.

Advanced synchrotron radiation and neutron tools are ideal for:

- Probing nanomaterial properties of individual particles, to image electrodes, and to observe the distribution of various species, their diffusion, the nature of interfaces, the presence and development of defects. In order to characterise the materials involved in hydrogen production, storage, and use, one needs atomic- and molecular level information on structure, hydrogen diffusion, and inter-atomic interactions, as well as the nanoscale and macroscopic morphologies that govern their useful properties. Neutrons are of great value for investigations related to catalysis, membranes, proton conductors, hydrogen storage materials and processes related to hydrogen production, storage, and use.

- Characterising energy-related nanomaterials under realistic operating conditions of energy converters (operando mode), e.g. nano-sized catalysts at demanding temperature conditions, electrode materials in corrosive environments, electro-catalysts at high potentials, coatings employed in thermochemical converters (combustion engines) and electrochemical converters (e.g. fuel cells).
- Studying crucial elementary steps of energy conversion, e.g. formation and breaking of chemical bonds, charge separation, and charge transfer. These events occur on a very fast timescale, at a surface, or involve minority species, hence very small concentrations of active species. In order to observe these processes, femtosecond pulses of extremely high brightness are required. These requirements can be fulfilled at an X-ray Free Electron Laser (X-FEL) facility. The facility for time-resolved studies on nanomaterials for energy should be associated with one the X-FEL sources.
- Evaluating material structures and accurately characterising them at various timescales and spatial scales from atoms (nm) to millimetres. In complex systems, this requires the availability of a comprehensive set of cutting edge instruments at high brightness sources, equipped with sensitive detectors. Methods include x-ray absorption spectroscopy (including EXAFS and XANES), x-ray and neutron diffraction techniques, including small angle scattering (SAXS and SANS), and many others. An efficient combination with fast data collection and high spatial resolution allow a mapping of experimental set-ups. Crucial are the availability of facilities for sample preparation / conditioning under extreme conditions of temperature and pressure, and measurement set-ups where samples and devices of technically relevant size can be investigated.
- Validating the multi-scale and multiphysics simulation codes (ranging from ab-initio to functional properties simulation), the use of which is expected to become more and more prominent in the field of material design.

Role of synchrotron radiation and neutrons for new technologies

Synchrotron radiation and neutrons will play an important role in the breakthroughs achieved in a large range of new technologies: energy carrier products, advanced energy conversion, storage and transport and energy saving (see Fig. 11.5.32).

Biofuels

- Improve the process for transformation of plants into biofuels;
- Understand the enzymatic process;
- Adapt and develop catalysts;

- Structure determination of active species at various scales from atomic to molecular;
- Follow the catalytic transformation of plants into bio-fuel (in-situ and in operando);
- Understanding of enzymatic processes for further adaption and development of catalysts.

Nuclear fission

- Develop new materials resistant to high temperatures, radiations and corrosion, as nanocomposite ceramics, cermets;
  Improve the life time in avoiding the occurrence of cracks;
- Detect crack initiation and propagation by nondestructive techniques;

- Structure determination and analysis of defects;
- Study of defect propagation under different stress and irradiation conditions (in-situ techniques);
- Chemical composition of defects.

Nuclear fusion

- Develop new materials resistant to very high temperatures, radiations and corrosion, as nanocomposite ceramics, refractories, refractory metals;
- Improve the life time in avoiding the occurrence of cracks;
- Detect the creation of defects by appropriate use of nanosensors;

- Structure determination and analysis of defects;
- Study of defect propagation under different stress conditions and irradiation (in-situ techniques);
- Chemical composition of defects.

Fossil fuel conversion

- The conversion will be directly improved by better catalysts;
- Find new low cost and performing catalysts;
- Reach the "zero emission" goal to protect the environment;
- Fully understand the catalytic processes at the atomic level;
- Develop microreactors;
- Design sensors to control the yield and emission of the processes;

- Characterise the chemical bond at the surface of catalysts and membranes;
- Detect and determine the nature of the intermediate species;
- In-situ and in operando studies;
- Structure characterisation at different scale from atomic to molecular;
- Analysis of stress states and morphology changes for diagnostics of nanostructured or nanosensor equipped coatings for life time prediction in service.

Solar cells

- An optimum utilisation of the solar spectrum through the coherent stacking of several solar cells with different band gaps;
- An alternative is to introduce intermediate levels in the band gap (MIB concept);
- The specific band alignment of the heterocontacts depends crucially on the particular crystallographic orientation of a grain and/or the chemistry at the interface;

- Control the morphology of the thin films and the interfaces;
- Development of nanostructured materials to better match the solar spectrum and enlarge the PV bandgap;

- Characterise the electronic, energetic and chemical structure of atomic layer interfaces;
- Provide structural information;
- Image lateral inhomogeneous work function distribution;
- Determine the local band gaps, barrier heights and their relation to the local chemical and structural composition;
- Obtain information on the local charge transfer dynamics and the excited states of nanoparticles.

Thermoelectricity

- Increase the temperature for the hot part, in designing new materials;
- Study the phase transitions, electron-spin and electron-electron interactions;
- Lower the heat conduction of the materials;
- Tailored synthesis methods for structured materials from nano- to macroscale;
- Improve the life cycle of the materials;
- Develop new interfaces to improve the phonon electron conversion;
- Find new, unconventional materials with good thermoelectric properties;

- Description of the structure at different scales;
- Study of the dynamic processes including structural changes and electron mobility;
- Study of the electron-electron and electron-phonon interactions on a nanometre scale during operation in order to point out new research strategies for materials with low heat conductivity and high electric conductivity;
- Imaging of interfacial reactions of thermoelectric convertors in operando.

H_2 production

- Improve the electrolysis process;
- Find performing catalysts for water photodecomposition;
- Understand the catalytic processes;
- Develop performing membranes for hydrogen purification;
- Develop new catalytic systems inspired by biological systems;

- Structure determination at the atomic and molecular level in order to improve electrolysis processes and to find suitable catalysts for water photodecomposition;
- Determine the morphologies at different scales;
- Study the functioning in the in-situ and in operando modes;
- Characterise the surfaces and interfaces;
- Determination of morphologies on different length scales i.e. membranes for hydrogen purification or studies of the sorption/desorption kinetics.

Fuel cells

- Find and develop new materials for the electrodes, the electrolytes and the membranes, functioning at the convenient temperature;
- Obtain better and cheaper catalysts allowing to easily use other gases than ultra pure hydrogen;
- Insure efficient ion and electron conductivities at the various interfaces;
- Understand the changes in the chemical bonds, the atomic and electronic structure;
- Characterise the cells in the in-situ or in operando mode;
- Precisely determine the ion diffusion processes;
- Obtain a better understanding of structure and transport properties of conventional membranes;

- Radiography and tomography of the cells (in-operando) to visualise the fuel cells and stacks in operation mode: species diffusion, phase stability and electrode-electrolyte interface changes;
- Determine the changes in the structure and oxidation states of the elements. Neutrons are especially performing in detecting the hydrogen atoms either in molecular hydrogen or in resulting water;
- Study of the catalytic processes – interactions between reactant gases and surfaces of catalyst) if natural gases are used (in-situ or in operando);
- Study the various interfaces either between the different parts, electrodes, electrolyte, current collectors, or inside them if they are on a composite form;
- Global characterisation in the in-situ or in operando mode.

Converter materials

- Depending on the system, improve the resistance to pressure, temperature or corrosion;
- Develop new tailored coatings with improved adhesion;
- Control the in-service evolution of the performances by diagnostics at the nanometer scales;
- Coatings with self-healing properties;
- Develop nanosensors;

- Information on stress state and morphology changes;
- Characterisation of the chemical preparation of nanocoatings and their application;
- Following of the performance in service;
- Structure characterisation at different scales, including the defects and their propagation.

Supercapacitors

- Develop high reactive surfaces;
- Better understand the surface interactions between charged species and electrodes;
- Improve the quality of the charge transfer;
- Find new materials with higher voltages;

- Structural characterisation at an intermediate scale (SANS and SAXS);

- In-situ and in operando measurements (dynamic studies) in order to probe the changes induced by the charge transfer in both the chemical bonds and the atomic structures;
- Precisely characterise the surface interactions and species diffusion.

Batteries
- Prepare new performing formulation in the nanosize, in order to improve the reactivity;
- Understand the reactivity at surfaces and interfaces;
- Fully characterise the chemical bonds;
- Model the behaviour and electrochemical characteristics by calculation approaches;
- Optimise the composite formulation and structure of the electrodes;
- Develop high conducting solid electrolytes;
- Improve the safety and lifetime;
- Reduce the cost of the materials and the technology;
- Probe the batteries and their components during the functioning;
- Mapping of the batteries (electrolyte and electrodes) to detect diffusion processes and inhomogeneities;

- Precise determination of the structure changes locally (EXAFS) and longer distances: identification of the key causes for performance fading (SANS, SAXS , diffraction);
- Characterisation of interfaces;
- Precise knowledge of the electronic states (XANES and PES) and, therefore, the electron transfer processes;
- Mapping of lithium diffusion (QENS) and composite electrodes;
- In-situ and in operando studies in using chemical dynamic studies (quick XAS and dispersive XAS);
- Identify the key points explaining the capacity fading and short live of batteries (defects, structure, diffusion).

H_2 storage
- Find new high performing materials with high specific area and porosity;
- Precisely determine the structural and electronic changes induced by hydrogen reaction;
- Understand precisely the sorption phenomenon of hydrogen ;
- Characterise precisely the physical and chemical bonds under different pressure and temperature;
- Study the dynamic of sorption-desorption processes;
- Reach very fast kinetics for sorption and desorption of hydrogen;

- Structure determination at the atomic and molecular level (x-ray and neutron diffraction, SANS and SAXS, EXAFS);
- Study the hydrogen sorption, desorption and diffusion (neutrons) in static and dynamic modes (in-situ and in operando studies);
- Determine the morphologies at different scales;
- Quantify the amount of hydrogen stored in the material.

Power transmission lines
- Precisely study the physics of electron transport phenomena at the nanoscale;
- Build composites and develop them at a high scale;
- Protect the lines against ambient conditions and corrosion by appropriate coatings;

- Physical studies of the electron transport phenomena in nanostructured composites;
- Structural characterisation of the composites from the nano- to macroscale;
- Imaging of the lines;
- Study the stability under severe conditions (in-situ experiments).

Light sources
- Prepare and develop new materials/alloys – at atomic scale – for white light production;
- Control the nanosize of the acting material particles;
- Fully understand the electron-hole recombination processes;
- Control the energy level and life time of excited states;

- Capture and analyse the excited states and electron path recombination of light active materials by very fast – highest time resolution) in-situ experiments;
- Determine the electron path;
- Precisely know the structure at different scales;
- Control the synthesis process;
- Produce and characterise nanometre thicklayers (CVD or similar techniques).

Insulation
- Develop materials with high specific area;
- Build composites and develop them at a high scale;
- Protect the materials against ambient conditions and corrosion by appropriate coatings;

- Structural characterisation of the composites from the nano- to macroscale;
- Imaging of the lines;
- Study the stability under severe conditions (in-situ experiments).

Strong light-weight materials
- Find new materials for transportation, much lighter than the existing ones;
- Insure the high resistance under severe conditions (temperatures, humidity, corrosion);
- Control the occurrence and propagation of defects;

- Structural characterisation of the materials from the nano- to macroscale;
- Imaging of the materials;
- Study the stability under severe conditions (in-situ experiments).

Conclusions and research strategy

The global and continuously growing energy problem will require a multitude of energy sources and priority research should include fuel cells and photovoltaic cells; solid-state lightening and batteries; modern and environmentally-friendly fossil fuel power stations and thermoelectrics; nuclear power; hydrogen generation and storage. This focuses research on new materials development, modern materials design and the most advanced modelling of materials properties. Great efforts should be devoted to nanomaterials science and technology; they offer great promises in realising breakthroughs in developing new energy technologies.

It is clear that the breakthroughs and discoveries in materials are essential to our ability to meet the exacting demand of any future energy scenario. Fabrication and the rapid and accurate characterisation of nanomaterials and nanostructures are central to our strategy in achieving these breakthroughs. Harnessing the benefits that result will require an intense collaboration between energy science, technology, industry, and specialists at large-scale synchrotron radiation and neutron facilities. The best would go through the creation of "Energy centres" in the proximity of large synchrotron and neutron facilities in order to bring together all major players (basic energy research, industry, synchrotron and neutron experts) and connect them closely with advanced simulation capabilities. This would best be realised if "Energy research centres" are developed close to large-scale facilities. These research centres should network and unite the most powerful facilities and brightest minds of Europe to advance a European research programme on nanomaterials using synchrotron radiation and neutrons for providing breakthroughs in the future energy scene. Such a facility has partly been recognised in the US by the construction of a Centre for Nanomaterials Science at the spallation neutron source at the Oak Ridge DoE lab in Tennessee.

Four types of requirements arise that will drive the development of new synchrotron radiation and neutron based research facilities:

- Increased structural resolution – to elucidate the atomic, nanoscopic, and mesoscopic arrangements that are crucial for enhanced performance;
- Increased spatial resolution – to directly image the functional units in physical space;
- Increased chemical resolution – to unveil the oxidation and binding state of the elements involved in the conversion process under investigation;
- Increased time resolution – to monitor in real-time the processes involved in the activation and deactivation of the novel energy converters.

	FUEL PRODUCTION	ENERGY STORAGE	ENERGY CONVERSION	WASTE MANAGEMENT
DIFFRACTION	State and dynamics of catalyst structure	Structure, phases of storage materials	High temperature materials, nanocomposites	Corrosion; advanced waste treatment
SANS/SAXS	Enhanced oil recovery; hydrates	Nanoporous materials, active carbons	Fuel cell and gas separation membranes	Clay materials
XAS	Catalyst nanoparticles, surface alloys	Redox processes in batteries, electrolytes	Thermoelectrica; in-situ characterisation of catalysts	Metal binding to sorbents, multi-barriers
SPECTROSCOPY	Catalytic reaction mechanisms	Electrode surface processes, superconductors	VUV spectroscopy of combustion processes	Identification of elements, speciation
IMAGING	Microreactors in operando	Phases and grains in complex alloys	Working fuel cell stacks, engines	Visualisation of slow diffusion processes

Table 11.5.1: Overview of the use of synchrotron radiation and neutron techniques in energy technology analysis.

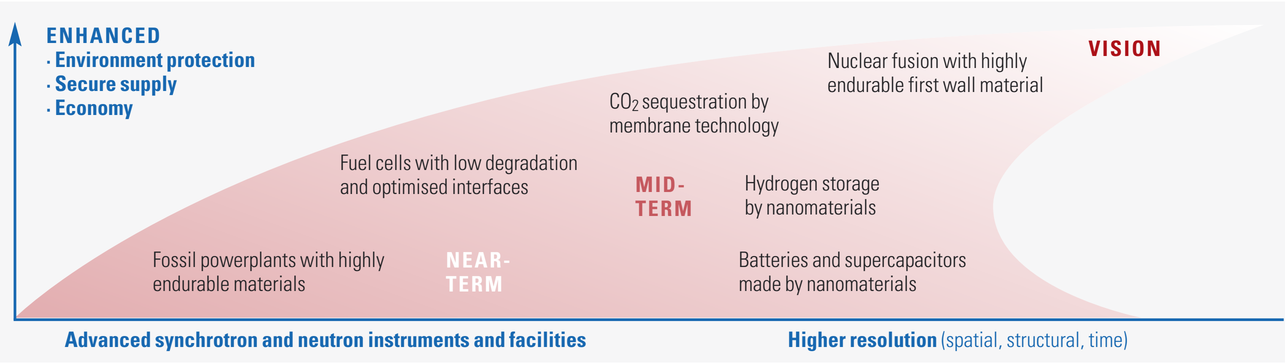


Fig. 11.5.33: Roadmap: Synchrotron radiation and neutron instruments for breakthroughs in future energy conversion and storage technology.

Pursuing these four goals in parallel (albeit, in part, in a task-sharing mode between different facilities) will represent an extremely challenging task, which may correspond to the development of a new generation of synchrotron and neutron sources. Although demanding, the provision of such powerful tools will without doubt pay off in terms of substantial advances towards a more sustainable energy system.

Table 11.5.1 highlights specific research needs on nanomaterials for fuel production, energy storage, energy conversion, energy saving and waste management, where synchrotron radiation and neutrons are essential in order to make further progress.

Fig. 11.5.33 gives the prospective use of synchrotron radiation and neutrons in energy technologies.

11.5.7. NANOMETALLURGY

Nanocrystalline metals are metallic materials, in which at least one internal length scale is smaller than 100 nm. Nanostructured metallic materials exhibit at least one external length scale smaller than 100 nm. Depending on the geometric complexity, this can range from thin films, nanowires to nanorods and nanoparticles, all of which have a potential use in nanoelectronics and nano-electromechanical systems.

Nanostructured metals are currently in use and gain more and more technological importance as the device dimensions are continually being reduced in microelectronics, sensors and actuators as well as in the coatings industry (see Fig. 11.5.34). Here, the optimisation of materials properties such as resistivity, reflectivity, electromigration resistance, barrier properties, interfacial toughness, fracture toughness, yield strength and tribological properties. Nanocrystalline metals, on the other hand, barely have a technological importance as the most promising processing routes; electrodeposition and severe plastic deformation yield only limited maximal sample sizes. They are, however, an ideal vehicle to study internal confinement effects on macroscopic mechanical behaviour and also provide a link to the understanding of the deformation behaviour of bulk metallic glasses, which currently also receive increased attention not only in the academic, but also the industrial field.

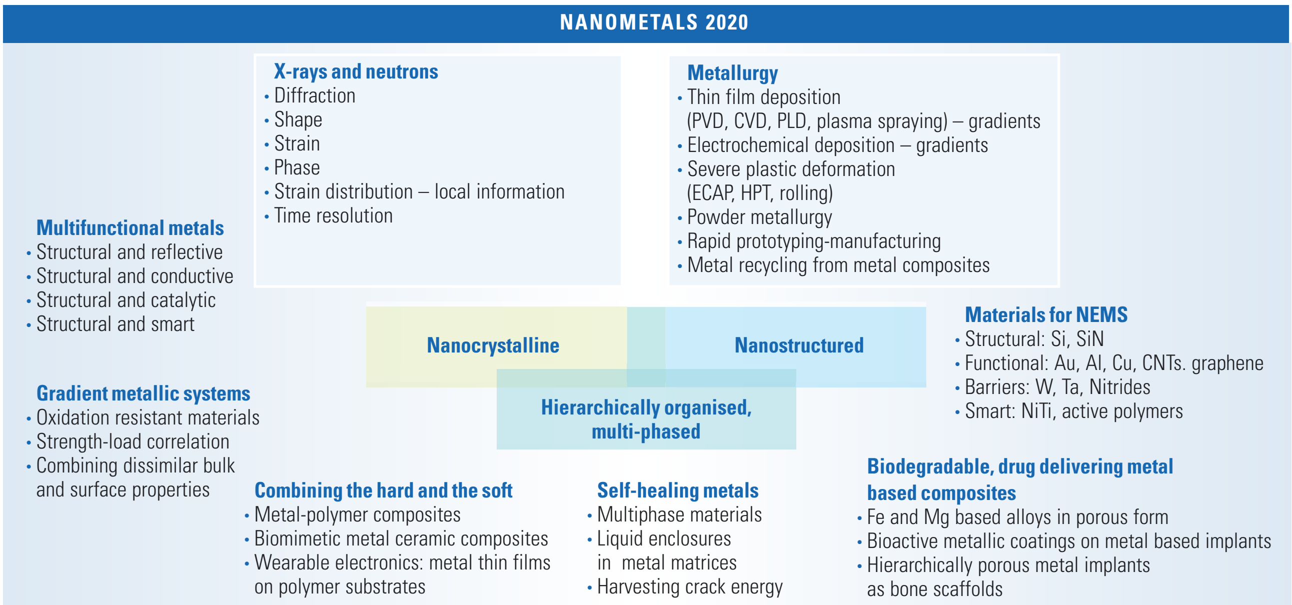


Fig. 11.5.34: Nanometallic materials and metallurgy

11.5.8. TRANSPORT TECHNOLOGY

The automotive and aerospace industries are torn between trying to reduce costs on the one hand and, on the other, dealing with the high price of performance-enhancing technology and environmental and legal compliance. There is a need for new materials to meet the challenging requirements of next generation aircraft. Nanotechnology seems to have the greatest potential for innovation and maintaining sustainable growth in this increasingly important sector. Within 5 to 10 years, mature, self-assembled, multi-functional nanostructured materials will be available to safely and affordably enhance aerospace applications. To summarise, the key issues in the land and air transportation industry are shown in Fig. 11.5.35. Fig. 11.5.36 highlights – as a reference – the requirements for future air gas turbines.

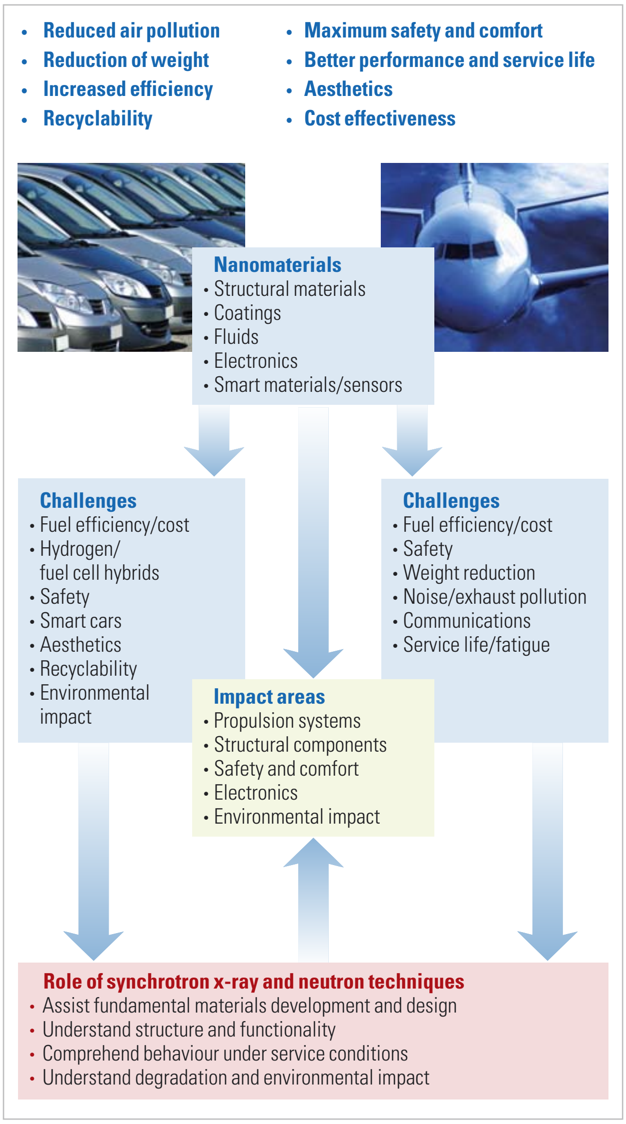


Fig. 11.5.35: Key issues in land and air transportation.

The requirements for nanomaterials to operate in aero-engine environments will be extremely stringent, the more so because they must outperform the most advanced engineering metallic alloy systems that are currently used in these applications. Failure cannot be tolerated in aircraft engines because of the severe consequences, but likewise the lifetime reliability must be such as to give 30,000 hours of operation. Fig.11.5.36 summarises the challenges faced for aero-engine components.

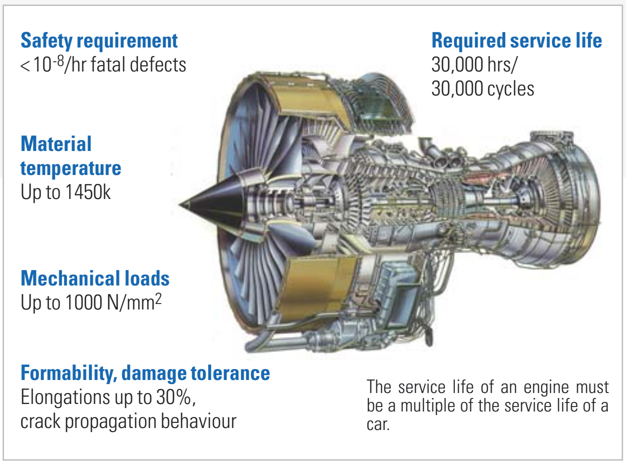


Fig. 11.5.36: Overview: Nanomaterials specifications in future aeroengines.

Research and development challenges on nanomaterials (see Fig. 11.5.37)

Almost all components in aircraft and road vehicles can and should be improved by nanotechnology, and the greatest impact in the near future is expected in the following areas:

- Advanced materials and structural technologies, for new, environmentally benign and corrosion resistant materials, and composite wrapping materials to reinforce older structures;
- Improved high-temperature alloys and coatings for supersonic, hypersonic and orbital craft (see Fig. 11.5.37);
- Energy, propulsion and environmental engineering for an improved transportation service that is cheaper, more energy efficient, and environmentally-friendly;
- Sensing and measurement technologies, making transportation safer and more reliable by: detecting obstacles to moving vehicles; route planning and speed setting according to weather patterns; changes in development resulting from transportation; and reductions in emissions of greenhouse gases and other system products. Non-destructive evaluation techniques using advanced sensor approaches will become more important as the physical infrastructure of the transportation system grows older, and has to be replaced;
- Analysis, modelling, design and construction tools, which will enable system planners to experiment with alternative system configurations, predict the performance of those systems, assess the

OVERVIEW NANOMATERIALS CHALLENGES IN TRANSPORT

NANOMATERIALS
Structural materials
Coatings
Fluids
Electronics
Smart materials/sensors

CARS

POWER TRAIN ENGINE – Research needs

Nanomaterials specifics
- Nanostructured protective coatings: thermal barrier – wear – corrosion resistant
- Nanofilters for particle free exhaust gases
- Nanopore fuel filter
- Nanoscale materials for catalytic conversion
- Nanomaterials based hydrogen storage
- Solar – Fuel cells/batteries with nanocomposed structures
- Ceramics with nanograin size
- Nanotube polymer composites
- Lubricant free power train
- Nanostructured sensors: gas- and liquids and in weld controls
- Magnetic materials
- Power electronics and optics

- Nanotribology
- Nanolubricants for reduced power losses
- Nanoreinforced steels for reduced weight
- Nanocoatings for reduced wear

FRAME – Research needs

Nanomaterials specifics
- Nanostructured polymer composites/fibres
- Nanoparticle coating for self-cleaning
- Scratch and dust resistant coatings
- Nanoparticles for wear resistant adherent tires
- Shape memory polymers
- Polymers with miniature sensors
- High strength – light weight carbon nanotube composites

- Light-weight nanomaterials
- Joining methods for nanoreinforced metallics
- Engineering damage tolerance at the nanoscale
- Corrosion-resistant nanomaterials
- Enhanced paints systems
- Easy to remove paint systems

AIRPLANES

POWER TRAIN ENGINE – Research needs

Nanomaterials specifics
- Nanodispersion strengthened metal alloys
- Light single crystal materials
- Nano MMC
- Nanostructured protective coatings:
- Sulfidation, erosion, fire, thermal barrier, tribology
- Low friction coatings
- Hybrid materials
- Gradient materials
- Reinforced materials
- Designed microstructures:
- Nanoscale processing and modelling
- Multi-functional materials for adaptronic designs,
- High temperature nanofunctional materials for sensors and actuators
- Smart intelligent materials

- Damage – failure analysis
- Nanojoining
- Nanotribology
- Nanocreep – nanolow cycle fatigue
- Crack initiation
- Development of high temperature,
- High strength steels with reduced density
- Nano NDT developments
- Cheaper alloy constituents
- More cost effective manufacturing
- Computational materials design and process engineering
- Life time models
- Standardisation: pore

FRAME – Research needs

Nanomaterials specifics
- Intelligent coatings
- Conductive coatings
- Self-repair adhesives
- Carbon nanotubes reinforced resins
- Nanoparticle reinforced MMC
- Metal-ceramic nanostructured composites
- Nanoparticle reinforced Mg-alloys

- Light-weight nanomaterials
- Joining materials and methods for nanomaterials
- Engineering damage tolerance at the nanoscale
- Fatigue of nanomaterials
- Corrosion-resistant nanocoatings
- Easy to remove decal systems

ROLE OF SYNCHROTRON X-RAY AND NEUTRON TECHNIQUES
Assist fundamental materials development and design
Understand structure and functionality
Comprehend behaviour under service conditions
Understand degradation and environmental impact

Fig. 11.5.37: Car and airplanes opportunities for nanomaterials.

impacts of those systems, and develop design improvements in one integrated process;
- New computer, information and communications systems for planning, design, development, maintenance, management and control.

The development and implementation of improved structural components are followed by components with enhanced material functions (smartness), increasing comfort and flexibility, and higher cost efficiency (see Fig. 11.5.38). Advances in the hydrogen economy are also anticipated in the medium term to long term, and these will revolutionise the transport infrastructure. These developments will provide the platform for revolutionary new designs in the long term.

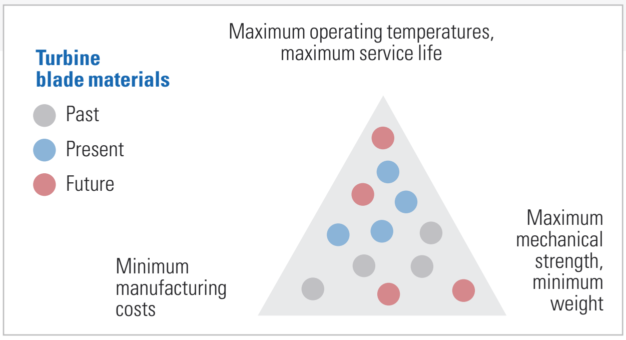


Fig. 11.5.38: New materials and manufacturing processes for gas turbines.

Role of synchrotron, x-ray and neutron radiation

In order to achieve fundamental breakthroughs in the underpinning technologies for our transport systems, advanced characterisation techniques will be required alongside conventional research tools to tackle the complexity over a range of length scales in terms of understanding and utilising (nano-)structure and functions of new materials. In particular, understanding the dynamics and functionality of new nanomaterials, ideally under service conditions (in-situ) and in real-time, is an area of research and development where traditional laboratory testing cannot provide the answers. In short, synchrotron radiation and neutron research have the capacity to impact strongly on the understanding of the life cycle of nanomaterials:

- Synthesis of new materials: light-weight structural materials, fuel cell materials, hydrogen storage materials and process engineering;
- Characterisation of engineering properties: Nanocreep, fatigue, crack initiation, nanotribology;
- Design and construction: nanojoining, NDT methods for nanomaterials;
- Quality control: identifying defects and characterising their initiation and propagation
- Structure and functionality;
- Behaviour under service conditions, including mechanisms of degradation and failure;
- Environmental impact.

Recommendations

The creation of research synergies and a closely coordinated effort of the materials science community will: pave the way to major breakthroughs in nanomaterials science and technology, ensure knowledge and technology transfer, and boost future competitiveness of Europe in the area of transportation in line with the Lisbon agenda. The necessary research consortia must involve academia and industry as well as the large scale synchrotron radiation and neutron research institutes.

Key to this will be the creation of partnership centres (GENNESYS Technology Centres of Excellence) at selected facilities. Successful implementation will require some adaptation by industry to work more closely with academic/large-scale facilities researchers, and flexibility by the large-scale research facilities towards industrial practices and standards, as well as an appreciation of the intrinsic value of applied research and the fact that industry timescales and research budgets are often highly restricted. Industry will benefit from the training of its staff in new technologies and the generation of a lead in research. Industrialists will be encouraged to disseminate the basic science findings of the research, but can retain the intellectual property of their designs and developments.

The obvious benefits lie in the creation of new nanomaterials and innovative technology, increased competitiveness within Europe, exchange of knowledge and skills between universities and industry, and the creation of an ideal fertile environment encouraging entrepreneurship and competitiveness.

Strategy and European research technology

This should comprise four directions:

- Development of high-performance nanostructured materials: metallic, ceramic, polymeric, coatings and composites; smart nanomaterials;
- Nano-engineering design: nanojoining, nanomachining;
- Fabrication of components from nanomaterials: e.g. turbine blades;
- Reliability of nanomaterials-based components in service: Creep and fatigue resistance, crack initiation and propagation, corrosion behaviour.

11.5.9. ENVIRONMENT

Sustainable development is now a fundamentally established fact, i.e. the growth we experienced at this time in developed countries can not be generalised worldwide without dramatic consequences for future generations. Nanosciences and nanotechnologies will play a major role with respect to this challenge we have to face, from both sides:

- Positive impacts because solutions provided by new opportunities at the nanoscale are able to open doors for new solutions for air, water or soil use, reuse or remediation, leading to a cleaner and healthier environment and way of living for every citizen, and a fair economy even in the developing countries;
- Positive impacts because it will help in the design of new materials, new processes with the generalisation of the green chemistry principle of "maximising atom economy" leading to less energy needs, less waste, less raw material, transportation reduction, risks reduction, and the "reuse" concept of "industrial ecology" in which waste of a process can be recycled as an input for another process in a local place;
- Negative impacts also because it is expected that the development of nanotechnologies will lead to a bigger production of products containing nano-objects (free nanoparticles) which alerts the citizen on the risk of unintentional release of those nanoparticles in the environment all along the life cycle of the product and their potential toxicity on the quality of the environment, employees and citizens' health.

From a practical point of view, environmental nanotechnology can particularly help in the following application fields:

- Supply of clean water for the world in a cheap and efficient matter; treatment of groundwater and waste water;
- More efficient catalysts to help reduce industrial and vehicle emissions and indoor/outdoor air purification;
- Cleaning and restoration of affected and polluted natural resources (water, air, soil);
- Monitoring the state of the environment through cheap real-time pollutant analysis using low-cost sensors and biosensors;
- Methods of CO_2 sequestration by reaction with nanostructured minerals;
- Develop processes for a safe geological disposal of nuclear waste, with methods acceptable for society;
- Understanding of the multiples ways of toxicity (direct and indirect) a nano-object can exhibit in its local biological environment (dispersion, effect, toxicity, remedy).

In this context, the key success factors will be to understand the complexity of the interactions that occurred between nano-objects, macro-objects and living objects (human or vegetal). It is expected by scientists that an interdisciplinary approach will be the only one that could bring a comprehensive understanding of a so complex interaction. In addition to new interdisciplinary approaches, one will need new tools, new lenses, to understand those mechanisms at the nanoscale level, from a static and dynamic point of view, and their consequences at the macroscale level. Thus, the role of synchrotron radiation and neutrons is essential for understanding basic interaction mechanisms and the characterisation of nanostructures and interface properties, especially for materials under extreme solicitations (reactive medium, biological growth medium, high pressure and salinity).

Improvements in advanced analytical technologies are of first priority, for instance in µEXAFS, µXANES, µXRD, Light scattering, Neutrons scattering, SANS, SAXS, 2-D and 3-D imaging techniques, depending on the nano-object size and length of the interaction to access a "dynamical multiscale characterisation tool".

Table 11.5.2 summarises the most important breakthroughs expected in these domains.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
NATURAL ENVIRONMENT			
Develop environmental technology for soil and groundwater remediation, water treatment, air purification, pollution detection and sensing, more efficient resources and energy consumption	Development of new materials with superior reactivity and behaviour	In-situ studies of nanoparticles – structure and aggregation	Characterisation of local components and interfaces (µEXAFS, µXANES, NMR, XRD)
		Kinetic studies of chemical reactions at the surface of nanoparticles	Characterisation of local components and interfaces (µEXAFS, µXANES, NMR, XRD)
		Understanding complex interactions in dynamic systems	Time-resolved characterisation techniques. 2-D and 3-D imaging, tomography
Evaluate the risk of nanotechnology for humans and ecosystems	Reproduce the conditions simulating engineering strategies dedicated to decontamination problems and waste management	Understanding natural/man-made nanoparticles structure and behaviour in different medias	Characterisation of local components and interfaces (SAXS, SANS, EXAFS, XANES)
		Understanding nanoparticles-living cells interactions in real conditions	Characterisation of local components and interfaces (SAXS, SANS, EXAFS, XANES) – 3-D crystallography)

MAN-MADE ENVIRONMENT			
Maximising atom use in nanofabrication processes	Mastering rapid self-assembly processes with less raw material, less energy, less and reusable waste	Understanding the first stages of nucleation, growth and self-assembly of hybrid matter (mineral, organic, living)	Characterisation of local components and interfaces (µEXAFS, µXANES Time-resolved characterisation techniques. 2-D and 3-D imaging, tomography
Man-made waste reduction	Improve the biomass as raw material – develop biocatalysts for CO_2 binding and reduction	Better understanding of CO_2 and small molecules green chemistry	Characterisation of local components and interfaces (µEXAFS, µXANES Time-resolved characterisation techniques. 2-D and 3-D imaging, tomography
Management of man-made waste: Pollutant capture and reuse (CO_2 reduction an dCO_2 reuse)	Develop new solvent/sorbents capable of robustness with respect to trace impurities	Understanding liquid/liquid interfaces (wetting, nanofluidics both gas and liquid)	Characterisation of local components and interfaces (µEXAFS, µXANES Time-resolved characterisation techniques. 2-D and 3-D imaging, tomography
	Develop nanostructured membranes for CO_2 capture, separation and storage	- Patterning matter at the nanoscale, grafting new function on new structures of membranes (hybrid concept) - Understanding nanofluidics (diffusion)	Dynamical and structural characterisation of flow in structures (µEXAFS, µXANES, NMR, XRD) Neutrons scattering (water, H_2) 2-D-3-D chemical imaging techniques XRD with nanometer resolution X-ray tomography HESX, EXAFS, XANES Neutrons scattering
CO_2 sequestration	Better identification of nanomaterial substrates for long-term sequestration and release	- New concepts of structured material at the multi-scale, - Understanding long distance interactions	
NUCLEAR WASTE			
Status of nuclear fuels just after burn-up -Development of nuclear fuels with higher efficiency and improvement of direct disposal and reprocessing methods	Understanding physical and chemical processes at a nanoscale level	- 3-D investigation of porosity - Elemental and radionuclide separation - Chemistry composition of fission products - Structure, short range order and oxidation states of nanoscale domains	2-D-3-D chemical imaging techniques XRD with nanometer resolution X-ray tomography with chemical information HESX, EXAFS, XANES Access to specific beam lines equipped for radioactive materials
	Understanding corrosion of spent nuclear fuels (SNF)	- Surface dissolution processes at nanoscale - Redox processes at the SNF/groundwater interface - Formation, dissolution, gas and ion diffusion through corrosion layers	RIXS Surface scattering and glancing XAS techniques Access to specific beam lines equipped for radioactive materials
Develop glass matrices matching with new nuclear waste, and capable of resistance to long-term alteration	Composition, structure of nuclear glass of nanoscale domains	- Structure of amorphous glassy structure and crystalline nanoscale domains - Oxidation states – local order of radionuclides	2D-3D chemical imaging techniques EXAFS, XANES, XRD Access to specific beam lines equipped for radioactive materials
	Alteration of nuclear glass on a long-term scale in engineered materials and natural and archaeological analogues	Surface dissolution processes Influence of ligands Study of alteration layers	EXAFS, XANES, XRD with adequate sample environment
Develop new containers capable of radionuclide retention, mechanical and chemical strength on a very long term scale	Behaviour of container walls under realistic disposal conditions	- Nanoscale structure of containers before and after exposure, under typical disposal conditions	EXAFS, XANES, XRD with adequate sample environment Access to specific beam lines equipped for radioactive materials
	Understand corrosion processes of metallic containers	- In-situ investigation of corrosion processes - Chemical and physical investigation of corrosion products	2-D-3-D chemical imaging techniques XRD with nanometer resolution X-ray tomography with chemical information HESX, EXAFS, XANES

	Find more efficient backfill materials to restrict water and gas diffusion and reduce mechanical stress of containers	- Pore distribution - Radionuclide reactions - Investigation of colloidal radio-nuclides	SANS, SAXS, HESX Neutron scattering techniques Access to specific beam lines equipped for radioactive materials
Investigate the radionuclide migration processes in the geosphere and the hydrosphere	Properties of the highly heteroge-neous nature of geologic matrix surrounding nuclear waste Understand transfer of radionuclides into plants, food chain and man	- 3-D pore distribution - Mineral distribution at nanoscale - Microbial distribution - Radionuclide distribution - Structural and chemical character-isation of colloids	SANS, SAXS 3-D crystallography Neutron scattering techniques Access to specific beam lines equipped for radioactive materials
Investigate the radionuclide migration processes in the biosphere		Spatial distribution of radionuclides - at water/soil/root interfaces - in transport vessels and cell organelles of plants - mucous membranes, blood vessels, organs of mammals	2-D and 3-D chemical imaging techniques Neutron scattering techniques Access to specific beam lines equipped for radioactive materials
NANOPARTICLES IN THE ATMOSPHERE AND CLIMATE CHANGE			
Role of nanoparticles for air quality	Understanding the interaction ´ between aerosol chemistry and microphysical properties of aerosols	In-situ internal structure and interfaces of multicomponent aerosols: fume, soot carbon, organic particles, sulphates, nitrates, dust,.. and of bio-aerosols (viruses, bacteria, biological debris)	Characterisation of local components and interfaces (SAXS, SANS, EXAFS, XANES, XRD) Tomography Neutron H scattering With samples in relevant atmospheric conditions
Role of nanoparticles for climate change	Discover the formation processes of organic particles and aerosols pre-cursors	In-situ studies of organic particles (low volatile oligomers and polymers, PAH, oxidized particles...) and other aerosols, under variable conditions.	Characterisation of local components and interfaces (SAXS, SANS EXAFS, XANES, XRD) with samples in relevant atmospheric conditions – Nanotomography
		3-D chemical composition under in-situ conditions	High resolution mass spectrometry under VUV ionisation
		Real-time studies of the nucleation process of aerosols – surfaces studies – role of enrichment of ions	Characterisation of local components and interfaces (SAXS, SANS, EXAFS, XANES, XRD) with samples in relevant atmospheric conditions
	Understand the chemical aging of aerosols and the transformation processes of organic particles during the atmosphere lifetime	Measure the properties of particles and their interaction with water vapour and other gaseous components	Soft X-ray spectroscopy and other structural characterisation methods
	Understand the optical properties of organic aerosols	Measure optical properties of organic aerosols	Visible and UV-absorption
	Better understanding of organic nanoparticles in the ocean	Studies of interaction of organic particles in salted water	Characterisation of local components and interfaces (SAXS, SANS, EXAFS, XANES, XRD)

Table 11.5.2: Breakthroughs in the field of nanomaterials for the environment.

Natural and man-made environment

At the moment, public awareness about nanomaterials technology is limited. A transparent discussion of benefits and risks will help people reach a balanced view. This will result in a greater public acceptance which finally will enable society to profit from these technological developments, while, at the same time, to keep the risks under control. An overview of environmental nanopollution is given in Fig. 11.5.39 and Fig. 11.5.40.

Positive effects on the environment

Nanomaterials technology has the potential has the provision of:

- Clean drinking water; remediation of pollution in air and soil;
- More efficient energy conversion and energy storage;
- Reduced material consumption;
- Enhanced diagnostic possibilities and new ways to treat diseases;
- New therapeutic methods for the treatment of cancer;
- Ultrasensitive detection of substances in environmental medicine and food safety;
- Development of sensors for environment monitoring.

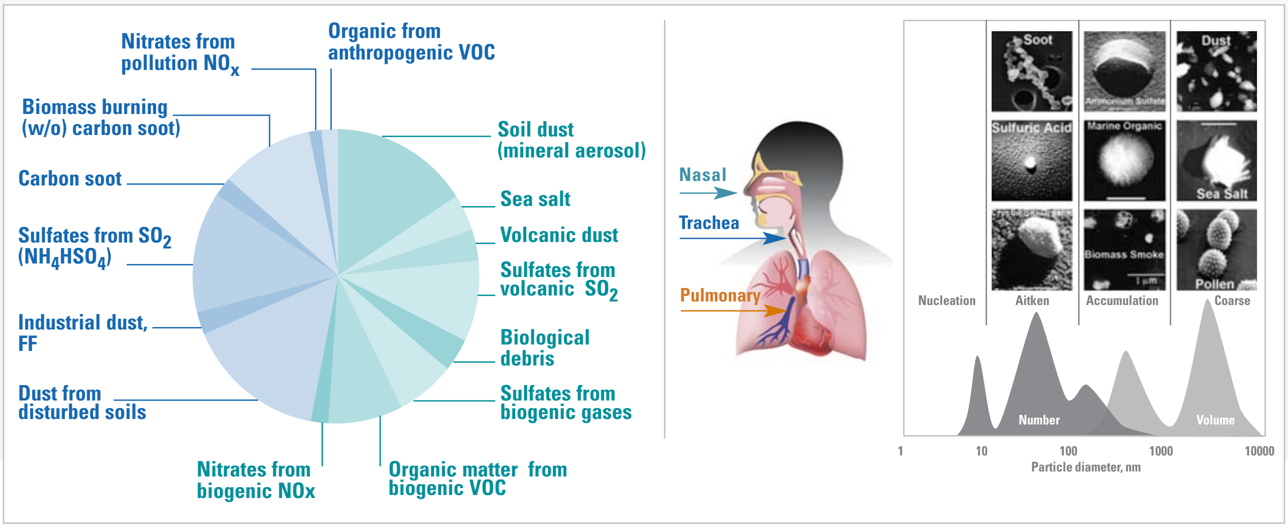


Fig. 11.5.39: An overview of environmental nanopollution.

Hazardous effects

The exposure to the environment has various origins:

- Industrial manufacturing of nanomaterials: range over the lifecycle of products and applications;
- Exhausts in transport systems: car (airbag gas generator) and airplanes;
- Nano's in polluted water, air, and soil;
- Nano's in food products (production processes, pesticides, extended shelf-life);
- Nanocosmetic products (active ingredients: transparent UV protection, tooth pasta);
- Sports articles e.g ski wax.

Nanomaterials for the remediation of anthropogenic activities on environment (Fig. 11.5.41)

- **Catalysts for the abatement of atmospheric pollutants emitted by industrial, transport and domestic activities.**
  Gaseous pollutants such as CO, NOx, VOC, unburned hydrocarbons, and aerosols of nanoparticles should be treated preferably at their source of emission: Highly active – poisoning resistant catalysts, electrocatalysts and photocatalysts are needed to reduce or eliminate them totally.

- **Nanostructured materials for the separation and capture of CO_2**
  Highly selective porous membranes for the separation of CO_2 from other gases (N_2) required for CO_2 capture.

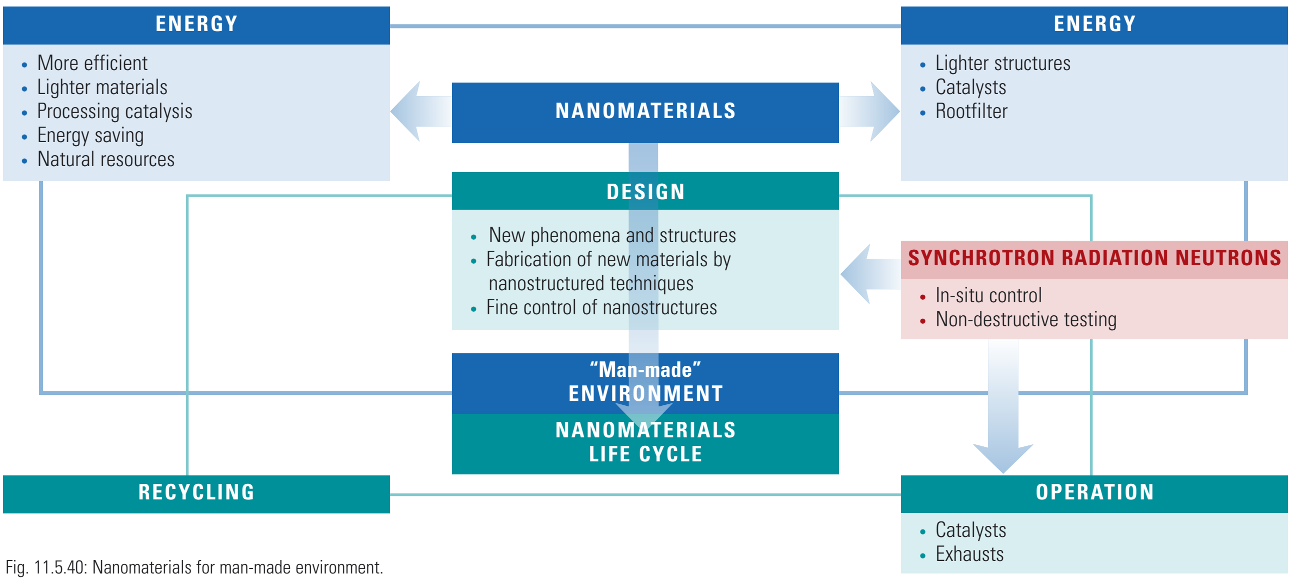


Fig. 11.5.40: Nanomaterials for man-made environment.

- **Adsorbent materials for water treatment**
  - Photocatalytic materials providing higher quantum yields for po luatant oxidation and microbialogic detoxification;
  - Highly porous materials with controlled pore size distribution and/or surface properties for selective absorption/adsorption of pollutants;
  - Bimetallic nanoparticles supported on high surface area oxide semiconductor for the oxidation of industrial organic pollutants in waste water.

Nuclear waste

Nuclear energy may have a place in future energy scenarios; the main concern regarding this type of energy is nuclear waste. The safe storage of nuclear waste is one of the great challenges for 21st century society. In order to guarantee safe storage, research should be directed to studies of the:

- Behaviour of ceramics and other nuclear waste forms under self-irradiation, including amorphisation, atomic-scale clustering, solid-state diffusion, and formation of microfissures and gas bubbles;
- Surface corrosion, redox processes and colloid formation at waste container/water interfaces;
- Transport of radionuclides in natural geomedia characterised by chemical microdomains;
- Biomolecular interfaces controlling the transfer of radionuclides to microorganisms, plants, animals and humans.

These processes have to be investigated with micrometre and nanometre resolution in order to improve the design of nuclear waste repositories and to provide society with reliable risk assessments. Key requirements for such research breakthroughs are synchrotron radiation and neutron techniques with appropriate micrometre- and nanometre-scale resolution, as well as the instrumental, administrative and legal conditions to perform research with hot radioactive samples at these large-scale facilities. Furthermore, the collaborative efforts of a wide range of specialists are required, covering fields from material sciences to geochemistry and medicine, and connecting universities with national and international research centres. These requirements are met by establishing a European Centre for Nuclear Waste Research located at a powerful synchrotron radiation or neutron source (see Fig. 11.5.42).

Nanoparticles in the atmosphere and climate change

The challenge for atmospheric science and climate science is to provide an understanding of the relationship between climate, air quality, and possible feedback within the Earth system. The process understanding of the interaction of aerosol chemistry and their microphysical properties are necessary for reliable predictions of climate and health effects of aerosol. Such an understanding is needed to accurately assess the impact of natural and man-induced change on the global atmosphere and to contribute to the development of political tools which enable a sustainable society.

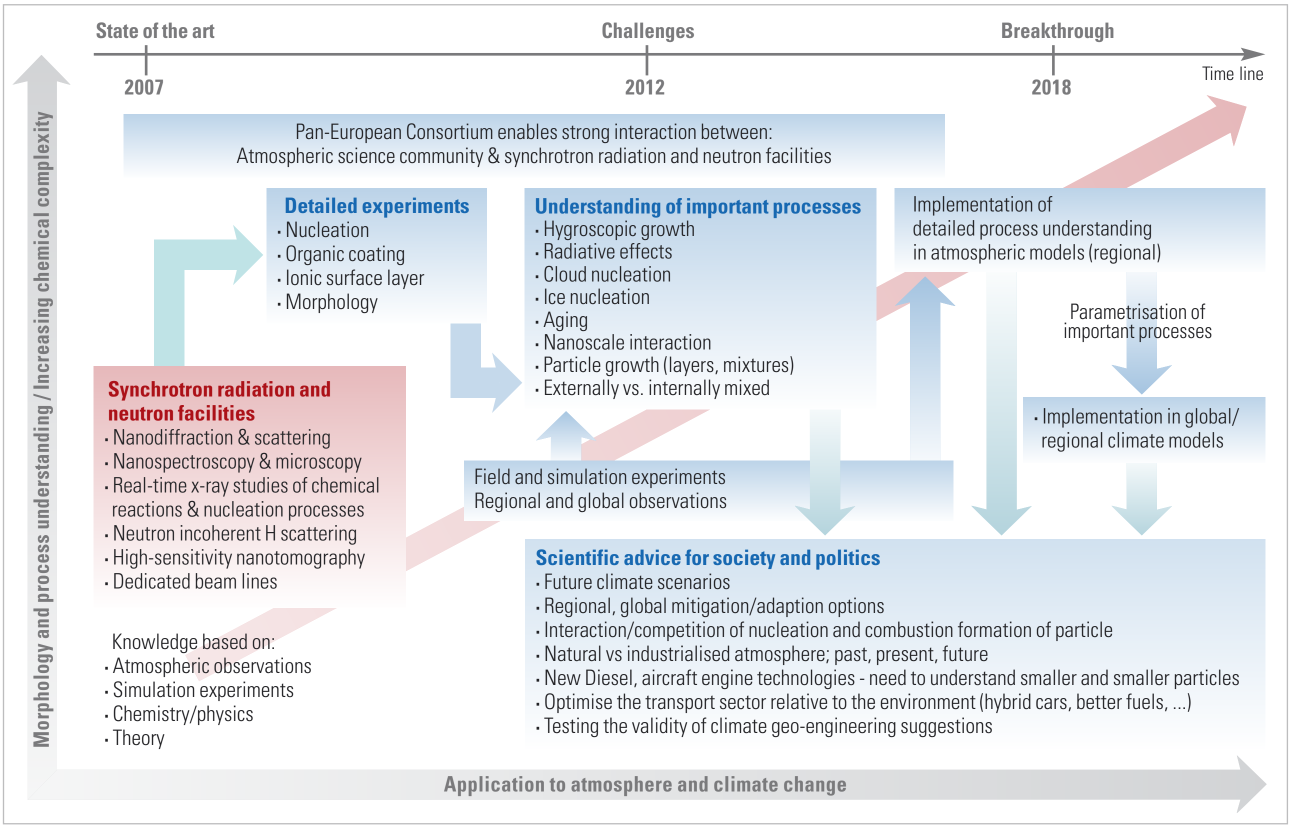


Fig. 11.5.41: Roadmap for future research on nanoparticles in the atmosphere.

There are two key attributes that distinguish the impact of aerosol on climate compared to greenhouse gases. Because aerosols accumulate in the submicron size range (resonant both with the wavelength of solar radiation and with the Kelvin effect, which controls the formation of cloud droplets), the radioactive impact of molecules condensed in aerosol particles on climate is amplified by about 1000 compared to molecules that remain in the gas phase. Furthermore, because those aerosol particles have an atmospheric lifetime of the order of a month, any changes in aerosol loading (anthropogenic or otherwise) have an immediate impact on climate, in contrast to greenhouse gases which continue to exist in the timescale of a century (see Fig. 11.5.43).

Significant gaps in our understanding of the interaction between aerosol chemistry and microphysical properties of aerosols hinder reliable predictions of climate and health effects of aerosols. Analysis, physical and chemical identification of atmospheric nanoparticles and their transformation processes are prime aspects of the future understanding of atmospheric chemistry climate interaction.

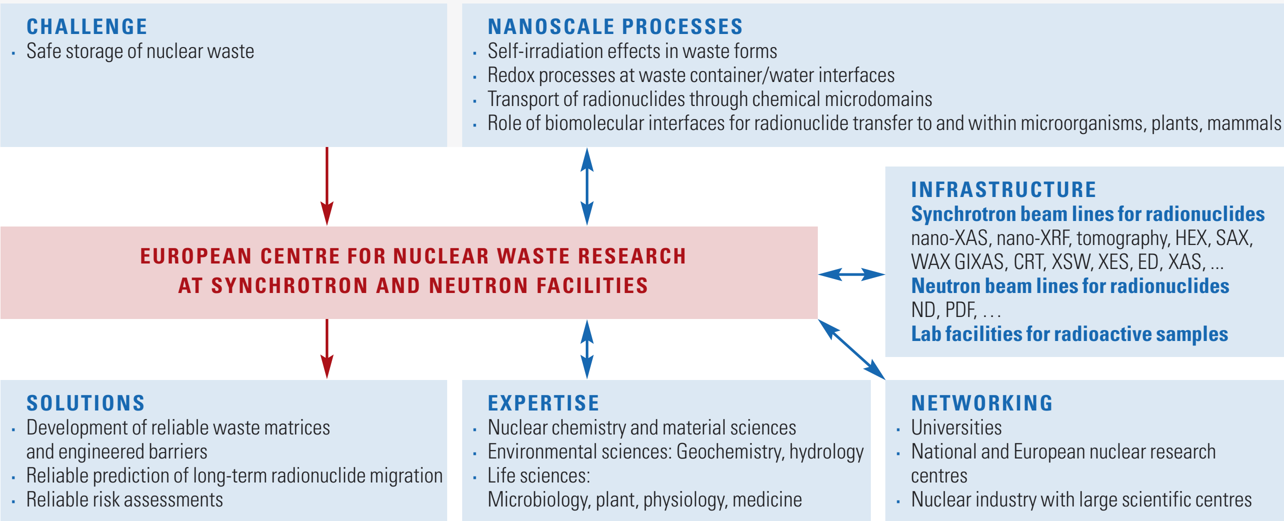


Fig. 11.5.42: Schematic representation of a European Centre for Nuclear Waste Research.

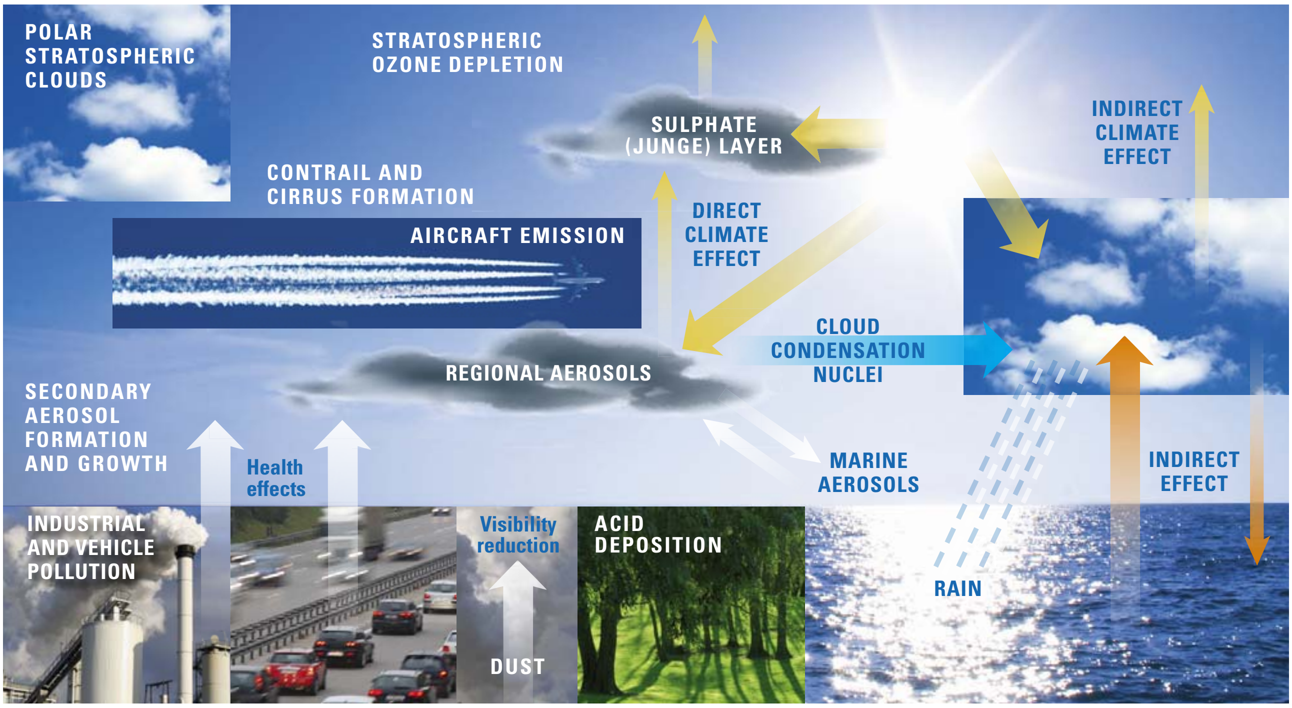


Fig. 11.5.43: Overview of atmospheric nanoparticles.

Advanced analytical tools provided at modern European synchrotron radiation and neutron facilities must be exploited in order to achieve a better microscopic understanding of the physical and chemical atmospheric processes which are triggered by aerosols. This requires dedicated experimental set-ups, which allow studying the structure and behaviour of aerosols under relevant atmospheric conditions in a systematic way from the formation of aerosol precursors to the ageing of aerosols, using:

- Nanodiffraction capabilities;
- Nanospectroscopy, microscopy and imaging capabilities;
- Real-time x-ray studies of chemical reactions in combination with optical light scattering and absorption;
- Quantitative neutron incoherent H scattering;
- High-sensitivity nanotomography in absorption or fluorescence mode;
- Ionisation via VUV-radiation combined with high resolution mass spectrometry;
- Development of dedicated beam lines and instrumentation which address the specific challenges of soft x-ray spectroscopy.

The synchrotron radiation and neutron facilities in Europe must develop the appropriate analytical technologies which provide the necessary microscopic understanding of all physical and chemical processes which are related to aerosols in our atmosphere. A pan-European consortium on "Nanoscience Issues in the Atmosphere and the Earth's Climate" must be implemented which coordinates inter alia the analytical needs (see Fig. 11.5.41). This will be one cornerstone for scientific advice for society and politics with regard to:

- Interaction/competition of nucleation and combustion formation of particles;
- New Diesel, aircraft engine technologies – understanding smaller and smaller particles;
- Optimisation of the transport sector relative to the environment (hybrid cars, aircraft engines, better fuels);
- Natural vs. industrialised atmosphere; past, present, future;
- Future climate scenarios;
- Regional, global mitigation/adaption options;
- Testing the validity of climate geo-engineering suggestions.

11.5.10. TOXICOLOGY

The expected contributions of nanotoxicology (Fig. 11.5.44)
Provide a service to governments and industries by (Fig. 11.5.45):

- Categorisation of nanomaterials based on standardised parameters that will indicate which nanomaterial and at what dose will pose risks;
- Recommend nanomaterials as 'Gold Standards';
- Reveal how novel nanomaterials can be used to improve or alleviate toxicological risks;
- Develop high-throughput toxicological tests to screen nanomaterials in-vitro and in-silico.

Synchrotron radiation and neutron facilities are needed for:

- Neutron reflectometry to determine surface characteristics of nanoparticles;

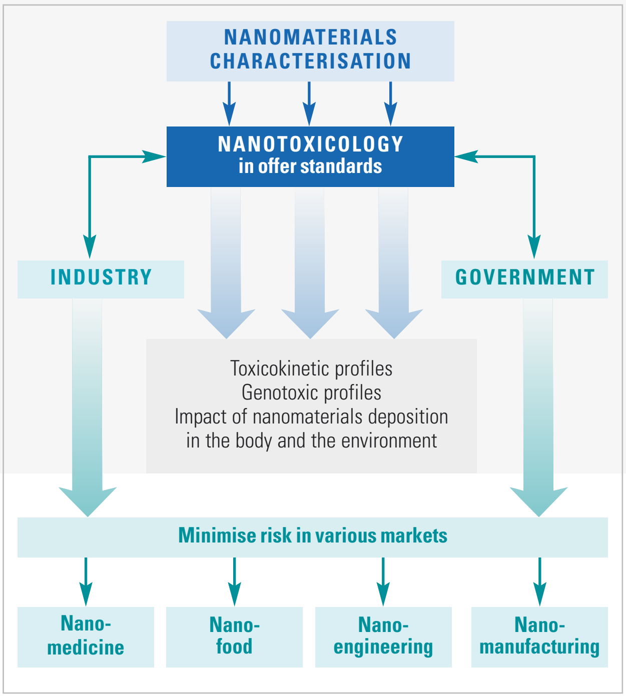


Fig. 11.5.44: The expected contributions of nanotoxicology.

- SAXS/WAXS to determine the structure of nanoparticles and nanocomposites;
- Time resolved x-ray and neutron sources to help determine the toxicokinetic profiles of nanoparticles in the body;
- Kinetics of inhaled nanoparticles at the cellular and mucosal (e.g. nasal, alveolar) level;
- Large-scale facilities in collaboration with centralised bio-informatics facilities to help establish nanoparticle structure-genotoxicity assays;
- High-end Electron microscopy facilities to establish morphological and structural characteristics of nanoparticles;
- Interaction of electrons, neutrons and other radiation particles with nanoparticles and the effect on their structural characteristics;
- Electron and neutron based techniques in the determination of nanoparticles in the environment and the impact of their accumulation in the food chain.

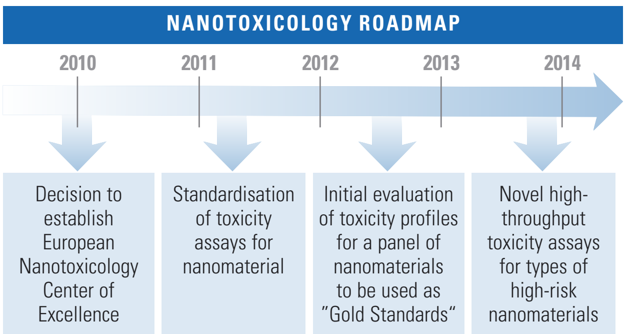


Fig. 11.5.45: Nanotoxicology roadmap.

11.5.11. ANCIENT AND HISTORICAL SYSTEMS

Archaeology, palaeontology, conservation and palaeo-environmental sciences all require a clever coupling of material characterisations at the macro-, micro- and nanoscales due to the chemical, structural and morphological complexity of objects and systems under study.

The relevant materials and their micro- and nanospecificities are summarised in the Table 11.5.3.

Breakthroughs are expected in these domains mainly through: i) the access to coupled macro- and nanocharacterisation tools, ii) strongly adapted support to the user communities, iii) in-depth interaction of synchrotron and neutron facilities with other LSF's (laser, microscopy, ion beam, dating facilities, etc). In addition, new instrumental and methodological developments are highly needed that involve complementary areas of research and development, particularly for 2-D and 3-D imaging. This is summarised in Table 11.5.4.

DOMAIN	TYPE OF MATERIAL	MICRO- AND NANO-SPECIFICITIES
Archaeology	Ceramic, glass, metal artefacts Stone tools, obsidians Organic remnants Pigments, rock art materials...	Micro- and nano-inclusions, micro- and nanophases
Palaeontology, archaeozoology and anthropology	Fossils, insects Teeth, bones, otholits, eggs Hairs, feathers, soft tissues Seeds, microflora, embryos...	Supramolecular organisation
Conservation and preventive conservation	Museum artefacts Coatings, protective treatments Built heritage...	Interfaces, grain boundaries, dislocations, texture effects Nanoparticles, nanoclusters, nanocolloids
Past environments	Sediments, speleothems, ice cores Microbial, plant and animal remains...	Complex 3-D morphology

Table 11.5.3: An overview of materials and their micro- and nanospecificities, as related to the study of ancient and historical systems.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
ARCHAEOLOGY			
Technological levels and ways of life of past societies	Resolve samples with a high level of heterogeneity and complexity	Clever coupling of nano- and micro-approaches	2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)
Reproduce past technologies and clarify the sequence of production steps to make artefacts	Follow-up kinetic reactions in controlled environment	Study a statistically representative number of samples (corpus)	Structural characterisation methods Adapted sample environment for structural and chemical analysis under controlled conditions
Degradation and aging mechanisms of archaeological artefacts	Resolve samples with a high level of heterogeneity and complexity	In-situ characterisation	
Predict the long-term behaviour of materials		Clever coupling of nano- and micro-approaches Study a statistically representative number of samples (corpus)	Structural characterisation methods 2-D and 3-D imaging techniques Surface sensitive characterisation methods
PALAEONTOLOGY, ARCHAEOZOOLOGY, ANTHROPOLOGY			
Study of ancient specimens of plant, animal and human morphology	Obtain high resolution morphological information	3-D non-invasive imaging	3-D imaging techniques
Observe specimens in amber, sediment, etc.	Obtain morphological information from samples embedded in opaque media	3-D non-invasive imaging	3-D imaging techniques
Study for evolutional and development models	Determine physico-chemical and mechanical behaviours from the study of specimens	3-D non- invasive imaging Clever coupling of nano- and micro-approaches	3-D imaging techniques 2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)

Understand mineralisation and fossilisation processes	Resolve samples with a high level of heterogeneity and complexity	Clever coupling of nano- and micro-approaches	3-D imaging techniques 2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)
Retrieve dietary and environment-related information Study DNA and other biomolecules preservation	Resolve samples with a high level of heterogeneity and complexity	Clever coupling of nano- and micro-approaches	2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)
CONSERVATION SCIENCE			
Develop nanoparticle-based conservation treatments Nanomagnetic gels for artworks consolidation that can be removed magnetically	Resolve samples with a high level of heterogeneity and complexity Investigation of nanosystems	Clever coupling of nano- and micro-approaches	2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering) Surface-sensitive techniques
Monitor the engineering of nanoparticle ensembles	Resolve samples with a high level of heterogeneity and complexity	Clever coupling of nano- and micro-approaches	2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)
Develop protective coatings from corrosion, water vapour	Follow-up kinetic reactions in controlled environment	In-situ characterisations	Surface-sensitive techniques Adapted sample environment for structural and chemical analysis under controlled conditions
Understand past artistic techniques and techniques	Resolve samples with a high level of heterogeneity and complexity	Clever coupling of nano- and micro-approaches	2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)
PAST ENVIRONMENT STUDIES			
Study climate records	High resolution trace element quantification	Obtain chemically-selective mapping at high resolution	2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)
Understand deposition processes	Resolve samples with a high level of heterogeneity and complexity	Investigation of nanoscale phase transition occurring during and after deposition	In-situ structural analysis
Investigate microbial, plant and animal remains from sediments	Obtain high resolution morphological information	3-D imaging	3-D and X-ray microscopy techniques
Complement dating techniques	Heterogeneity and complexity of the samples Analytical strategy preserving date validities	Clever coupling of nano- and micro-approaches	2-D and 3-D imaging techniques (fluorescence, absorption, diffraction, small angle scattering)
TECHNOLOGICAL REQUIREMENTS AND OTHER CONCERNS			
Optics and instrumentation Nanolocalisation, nanomarking	Optimise optics and instrumentation to the needs of nanocharacterisation	New instrumental developments	Develop advanced instrumentation at LSFs
Data storage Digitalisation techniques	Store very large amount of data from digitalised cultural heritage, archeological and palaeontological archives	New developments in recording, digitalisation and data storage	Contributions from LSFs to the development of microelectronics
Improve security and safety Prevent trafficking and looting	Combat artwork and archaeological object trafficking Secure museums, archive and storage environments	New developments in security (marking, etc.)	Contributions from LSFs to the development of security
Decrease cultural activities environmental impact	Develop energy-efficient systems	New development in environmental techniques	Contributions from LSFs to energy-efficient building

Table 11.5.4: An overview of breakthroughs in the field of ancient and historical systems.

The need for a European Centre for Ancient and Historical Nanomaterials

Beyond scientific and technological barriers, the strongest limitations are organisational ones. Ancient and historical systems require knowledge and development from many disciplines that would need to interact with each other in order to foster an efficient implementation of new analytical strategies and take benefit from specific scientific support and additional analytical facilities, for their access to large-scale facilities. Furthermore, stakeholders in the cultural and art world should strongly benefit from the competences and expertise of this Centre. The answer to these concerns is to set-up a Centre dedicated to ancient and historical nanomaterials, as schematically shown in Fig. 11.5.46.

This Centre will be organised with the following objectives:

- Develop innovative collaborative research activities on ancient materials and their environment, focusing on projects with an interdisciplinary character which cannot easily develop elsewhere and also on projects involving academic researchers and end users in culture and art;
- Offer various analytical instruments to prepare further studies with synchrotron and neutrons facilities;
- Develop new instruments and methods such as imaging, microscopy techniques and data processing methods, including modelling at the nanoscale on analytical methods, behaviour laws, mechanical models, etc.;
- Offer specific facilities for the storage and transportation of ancient specimens, objects, artworks and samples according to museum standards. Compliance with museum standards should be ensured for areas where artworks will be stored, even temporarily, or examined;
- Contribute to share the expertise among users, collect information, organise training events, disseminate to the end-users and to the public.

11.5.12. SECURITY AND SAFETY

The needs of security and safety research should be envisioned in the whole chain from fundamental, basic research to technological research, development, production and use of systems. At this time, the phases of development and industrialisation have not yet really begun because many efforts on the laboratory scale should be made first on the basic principles, using interdisciplinary programs, then on the identification of the technology, the proofs of concept and the laboratory mock-up. Additional challenges are brought by non-technical parameters associated to public acceptation and to ethical compromise between human being security benefits and citizen liberty reduction risks; because of the foreseen use of device/systems for human beings and in environment.

The importance of nanodevices can be paramount for the safety and security, because of the number of their features, such as (Table 11.5.5):

- Reduced volume, implying large-scale deployment without being noticed;
- Robustness to be used in every situations by virtually everybody;
- Reliability to provide repetitive significant answer for a given threat;
- Sensitivity: ideally for many threats, the detection of the first molecule/particle/pathogen is crucial in case of a crisis to determine as soon as possible the nature of the alarm, so that prevention/protection means can be deployed efficiently;
- Versatility.

Breakthroughs in nanomaterials for security and safety are expected from the combined advancement of nanotechnologies for electronics and optics, information, mechatronics, biology, cognition and energy. They are also expected in the capability of developing "systems of systems" capable of self-powering, local intelligence, combination of selectivity/versatility/sensitivity, rapidity, communication.

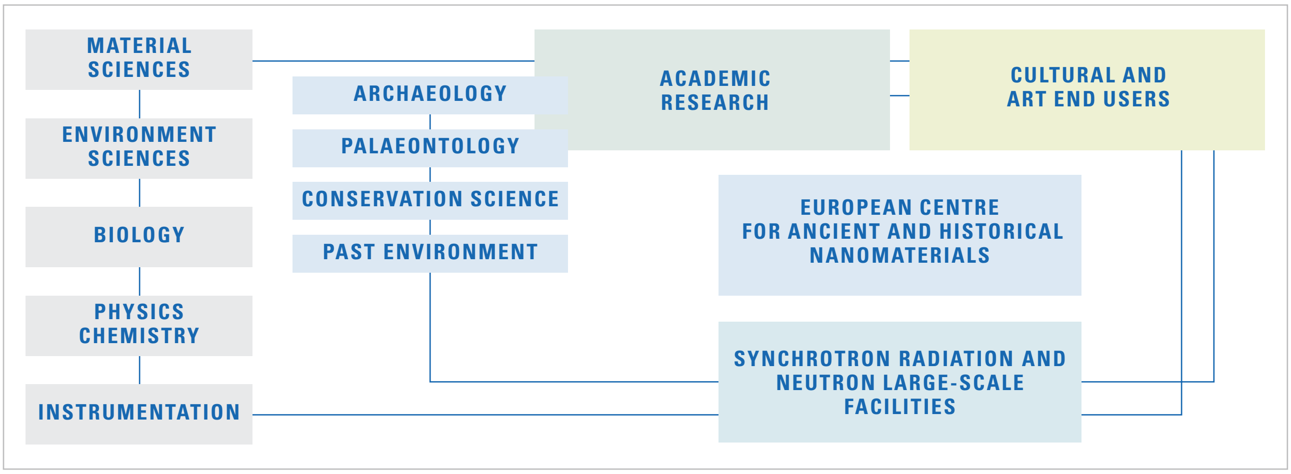


Fig. 11.5.46: Possible set-up for a Centre dedicated to ancient and historical nanomaterials research.

	SIZE REDUCTION	NEW PROPERTIES
Detection Identification Diagnosis	Sensors integration (clothes, real-time diagnosis, etc.) Sensors performance increase (parallelisation, etc.) Integrated systems	New sensors with better: • Performances • Convenience of use • Reagents free Bridging the gap between electronics and life sciences
Protection	Adaptive systems Communication Includes detection	More protection Multifunctional properties: • Detection and decontamination • Detection and therapeutic, etc.
Therapeutic prophylaxy	Facilitation of medical intervention (nanorobots for surgery, etc.) Facilitation of molecules delivery	New vectors New treatments
Decontamination – Rehabilitation	Communication Weight and volume reduction Ergonomy/comfort	New process Multifunctional properties

Table 11.5.5: Potentials of nanomaterials for security and safety.

GOALS	KEY BARRIERS	NEEDS	ROLE OF SYNCHROTRON RADIATION AND NEUTRONS
Obtain advanced micro/ nano- integrated sensors, actor nodes and systems	Obtain e-nose devices with enough sensitivity to compete with dog nose	NEMS substrate with DNA transmitter with different nano-objects (ex. carbon nanotubes)	Characterisation of local components and interfaces
	Create receptacles on metal with receptor molecules with a dangling bond attaching optical indicators	Nanogrooves and protein nanoarrays	Characterisation of local components and interfaces
	Obtain soft (bio) to hard (electronic) nanostructured systems	Tailored Lab on chips	Characterisation of local components and interfaces
	Chemical detection on large surfaces (walls, textile etc.)	Self-assembled gratings for nanodetectors	Characterisation of local components and interfaces
	Mechanical detection at the atomic level	Arrays of AFM	Characterisation of local components and interfaces
Understand the patho-genesis caused by threat agents and develop nano-systems for diagnostics, therapeutics and prophylaxis	Develop nano-actuation mechanisms	Nanodevices: ex nanoscale rotor/paddles	Characterisation of local components and interfaces
	At the genomic scale	Gene expression profiling	3-D crystallography
	At the protein scale	Specific proteins involved in selected pathologies (Proteomic)	3-D crystallography
	At the integrated scale	Nanodevices	Structural characterisation combining x-ray and NMR
Obtain protection nano-technologies for human use within a terrorist attack	Develop adaptative systems capable of communication and actuation	Specific integrated lab-on-chips devices	Characterisation of local components and interfaces
Obtain protection nano-technologies for safety applications	Develop materials with high resistance, improved friction, thermal conductibility or isolation capabilities or optical proper-ties, hydrophylicity or hydrophobicity	Nanocomposites Metal filaments, multiwall nanotubes Micelles systems with control of chemical release	Characterisation of local components and interfaces
Obtain nanosystems for decontamination and remediation	Develop nano-objects capable of toxin capture, avoid extra-contamination and easy cleaning methods	Cyclodextrines or mesoporous sensors devices	Characterisation of local components and interfaces

Table 11.5.6: The needs and role of synchrotron radiation and neutrons, as applied to nanomaterials for security and safety.

The success and the industrial penetration of applications will really be connected to the maturity of applications for mass market and their social acceptance. Early association of industry, through dedicated incentives for participation in research and development efforts is a must.

Priorities of nanomaterial research which give breakthroughs to the domain of "security, safety – reliability – and environment", are categorised as follows:

- Nanomaterials for advanced sensor and actor nodes and systems;
- Self-organised security chains, "system of systems concept";
- Nanomaterials testing methods (combined safety, reliability and security properties);
- Nanomaterials diagnostics (extremely small quantities, many substances including bio-pathogens or bio-inspired chemical agents);
- Monitoring of nanomaterials properties ("complex" analysis), e.g. long-term monitoring;
- Monitoring from very small to very large areas;
- Safety and reliability aspects of nanomaterials research;
- Clean-tech aspects of nanomaterials and nanotechnology for nanosecurity applications, their innocuity for long-term life cycle, their degradability or "reuseness/reusability";
- Combined social as well as technical aspects of security (and safety, and reliability);
- Risk analysis and risk management based on advanced nanomaterials knowledge.

Among these multiple topics of research, developing better sensors (especially with higher sensitivity, specificity, robustness and versatility), better protection (that includes physical protection but also prophylaxis and therapeutics) and better decontamination/remediation are amongst the main goals. In this respect, the role of synchrotron radiation and neutrons is an essential tool for 3-D patterning and characterisation of nanostructures and interface properties of a number of nanodevices and also for crystallography of bio-systems, biomolecule dynamics, from the nanoscale, via in vitro up to in-vivo characterisation. Table 11.5.6 summarises these needs and role of synchrotron radiation and neutrons.

11.6. KEY CHALLENGES FOR NANOSTANDARDISATION AND -METROLOGY

11.6.1. IMPORTANCE OF NANOSTANDARDISATION AND -METROLOGY FOR RESEARCH, INDUSTRY AND MARKETING

Nanostandardisation and nanometrology are key elements for research in nanomaterials, the development and industrialisation of nanomaterials technologies, and the realisation of the potential market for nanomaterials applications. In addition, standard reference materials and standard measuring techniques are vital in the evaluation of cosmetics and medical products and the formulation of regulations for occupational safety in laboratories and work space, as well as in environmental protection and toxicology.

The characterisation of nanomaterials is focused on standardised – valid, reliable, and comparable – measurements of physical, mechanical, electrical, and chemical properties and structures in three dimensions at the nanoscale. This demands special skills and advanced analytical equipment: synchrotron radiation and neutrons are the basic analytical tools for tomorrow's nanomaterials. The demands for standardised beam lines for neutron and synchrotron radiation experiments can be outlined as follows (see Fig. 11.6.1).

This chapter provides an overview of standardisation and metrology on nanomaterials for a wide range of industrial sectors, using synchrotron radiation and neutron sources (see Table 11.6.1). Standard measuring techniques and methods and reference materials should be developed for nanomechanical (creep, fatigue), physical (interfaces, tribology, friction, wear), chemical (surfaces), electronic and other properties. In-situ measurements at synchrotron radiation and neutron sources will have their places in the characterisation of nanopowders, particles, etc. during processing, at surfaces and interfaces, preparation of an evaluated database, service reliability and life time prediction studies etc.

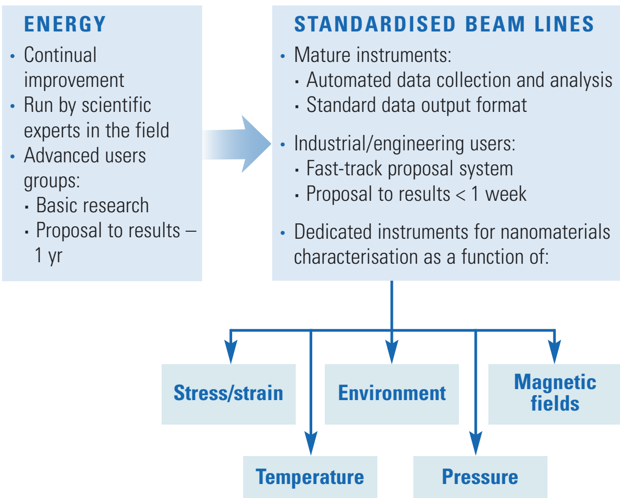


Fig. 11.6.1: The demands for standardised beam lines of synchrotron radiation experiments.

Information and communication	· Multi-layers/nanowires · Surfaces: atomic sites at silicon surfaces · Thin films and smart coatings · Magnetic nanoparticles · Nanoassembled materials · Functional surfaces and materials · Nanocomposites · Multifunctional devices (transducers) · Molecular and polymeric materials (sensors, organic semiconductors) · Dielectrics, magnetics
Chemistry	· Nanosyntheses and production characterisation · Surface textures · Nanostructured materials · Nanoparticles · Nanopowders
Catalysis	· Surfaces · Interfacial phenomena
Health and biomedical	· Functional Gradient Nanomaterials for biomedicine · Nano-biopolymer functional materials · Bionano actuator/molecular switch for biosensing · Nanoparticles characterisation/ safe use · Bioaffinity · Surface · Biodegradation
Mechanical engineering	· Nanostructured intermetallics · Nanostructured metal/ceramic/ polymer composites · Thin film actuators, sensors, NEMS · High temperature & corrosion resistant & smart coatings · Thermal barrier coatings · Functional surfaces and multilayer's · Nanomaterials for fuel cells · Insulating materials
Energy	· Polymer composites (particles and fibres) · Functional textiles · Multifunctional coatings · Crack resistant nanoceramics · Thermal gradient materials · Functional surfaces and multilayer's · Nanomaterials for fuel cells · Insulating materials
Transport – automotive and aeronautics	· Polymer composites (particles and fibres) · Functional textiles · Multifunctional coatings · Crack resistant nanoceramics · Thermal gradient materials

Table 11.6.1: Overview of nanostandardisation and metrology for industries using large-scale facilities.

11.6.2. NANOSTANDARDISATION AT LARGE-SCALE FACILITIES FOR MULTIPLE INDUSTRIES

Guidelines are given for the nanostandardisation, the experimental set-ups of nanomaterials and components for some important industrial groups:

Chemistry and chemical engineering: nanopowders and nanoparticles

Future nanomaterials research demands the knowledge of chemical composition, structure and function over multiple length scales with additional emphasis on dynamic properties and functions. Nanopowders and particles are systems with characteristic dimensions between 1 nm and 1 µm. In the future, regulations made by environmental protection agencies will influence products and processes containing nanoparticles. There is a great lack of standard reference materials and methods with respect to reliability, materials homogeneity, accuracy and precise quantification, and affordability. Standardised analytical tools for: nanoparticle size, surface, shape and composition are also required.

The small-angle, wide angle x-ray-scattering and extended x-ray absorption fine structure measurements (SAXS/WAXS/EXAFS), in combination with transmission electron microscopy (TEM) and scanning probe microscopy (SPM), are the most suitable techniques to characterise "standard reference materials" for all structures <100 nm. Information can be obtained on size distribution, shape, internal structure, porosity, surface, degree of crystallinity; composition for studies on synthetic; natural macromolecules; biomolecules (plastics, proteins, DNA, viruses); colloids and dispersions (metal and alloy nanoparticles, quantum dots).

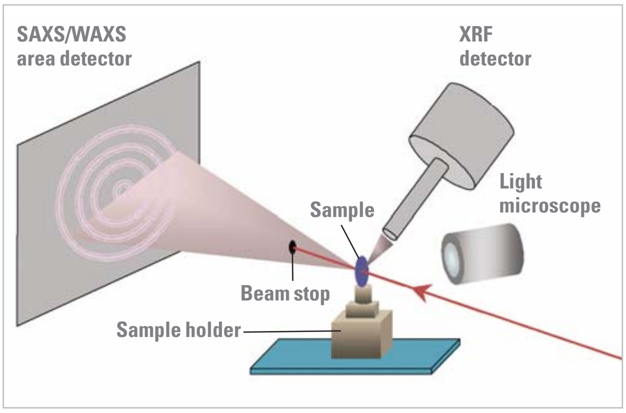


Fig.11.6.2: SAXS for nanomaterial reference studies.

Synchrotron and neutron based on SAXS/WAXS/EXAFS methods are the most promising techniques for "in", "at"-, and online "in-situ" process monitoring and advanced control strategies that create feed forward and back information, instead of end product testing and thus required for standard control processes, practices, and guidelines. A WAXS/EXAFS experimental set-up for the characterisation of nanomaterial reference studies is shown in Fig. 11.6.2.

Standard experimental configurations

The standardisation of the synchrotron experimental set-up for chemical reaction studies (e.g. catalysis, oxidation, sulfurisation, nitridation) is represented in Fig. 11.6.3 and Fig. 11.6.4.

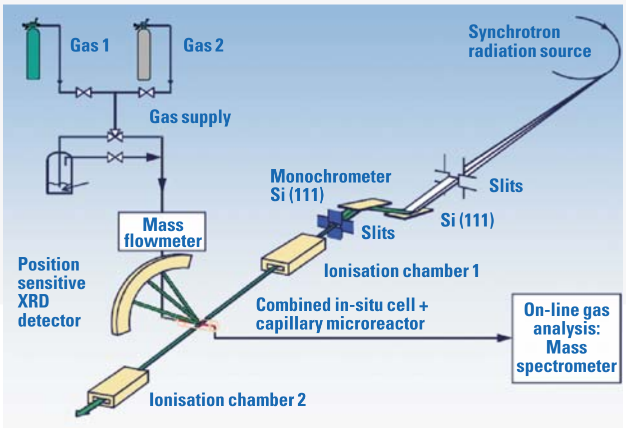
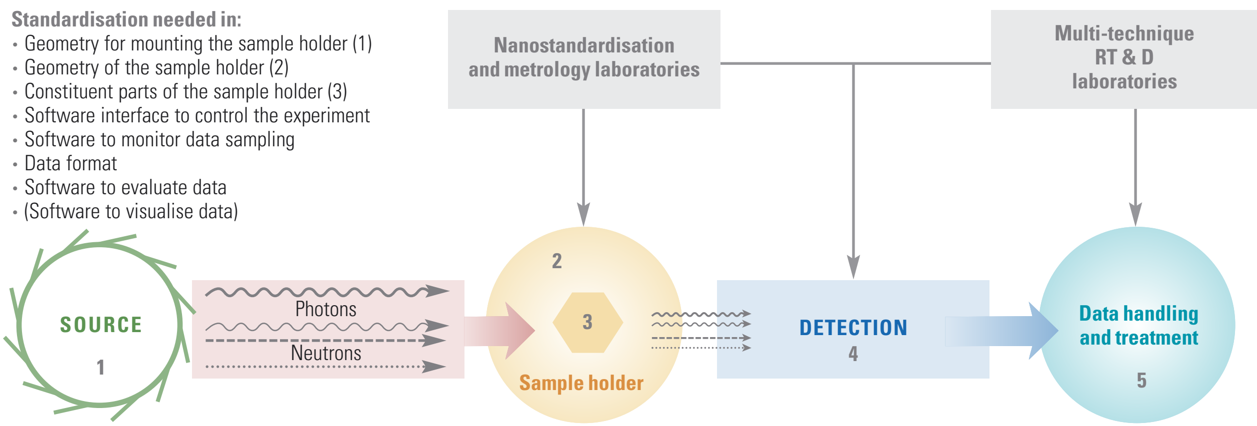


Fig. 11.6.3: Practical layout of an experiment with synchrotron radiation.

Nanomaterials metrology for health – bio- and medical applications (Fig. 11.6.5)

The biological response from biomaterials down to molecular therapeutic drug agents shows exquisite dependence on structural property. With nanomaterials, we are at the threshold of using materials which are able to converge and harness both these dimensional domains of therapeutic capability. Accordingly, there is a particular need to ensure that the sensitivity and reliability of characterisation is the highest magnitude, and certainly on a level that matches the high resolving power of biological systems – macromolecular, cellular or whole body. Without this, the interpretation of biological and medical outcomes of nanoparticle interactions and indeed their therapeutic become unreliable and merely descriptive.

Irrespective of whether a nanoparticle is polymeric, inorganic or metallic, it is necessary to have combined absolute measures of both bulk and surface properties; both determine bioactivity and subsequent fate. Industrial scale characterisation by x-ray scattering (SAXS/WAXS) and by neutrons has the potential to provide not only the necessary baseline measurements on nanoparticles (bulk porosity, surface spe-



Technique	Pressure range	Temperature range	Spatial resolution	Energy resolution Chem. sensitivity	Time resolution	Principle information	Sample restrictions
(Surface) x-ray diffraction SXRD	no limitation	no limitation	0.001 nm	a few eV/ anomalous scattering	sec to ns in pump-probe experiments	Crystallographic structure and morphology	(Optically flat surface) none
Grazing incidence x-ray/neutron diffraction GID	no limitation	no limitation	1 nm	a few eV/ anomalous scattering	sec to ns in pump-probe experiments	Near surface structure	(Optically flat surface) none
Extended x-ray absorption fine structure EXAFS	no limitation	no limitation	0.003 nm	0.1 eV/yes	milliseconds	Local structure, chemical environment	none
X-ray photo-electron spectroscopy XPS	< 13 mbar	< 900 K	–	0.005–0.3 eV/yes	seconds	Chemical bonding state	Conducting material
(Grazing incidence) Small-angle x-ray scattering GISAXS/SAXS	no limitation	no limitation	1–100 nm	a few eV/ anomalous scattering	sec to ns in pump-probe experiments	Particle size, shape, porosity	(Optically flat surface) none

Fig. 11.6.4: Standardisation of nano-oxidation experiments at synchrotron radiation sources.

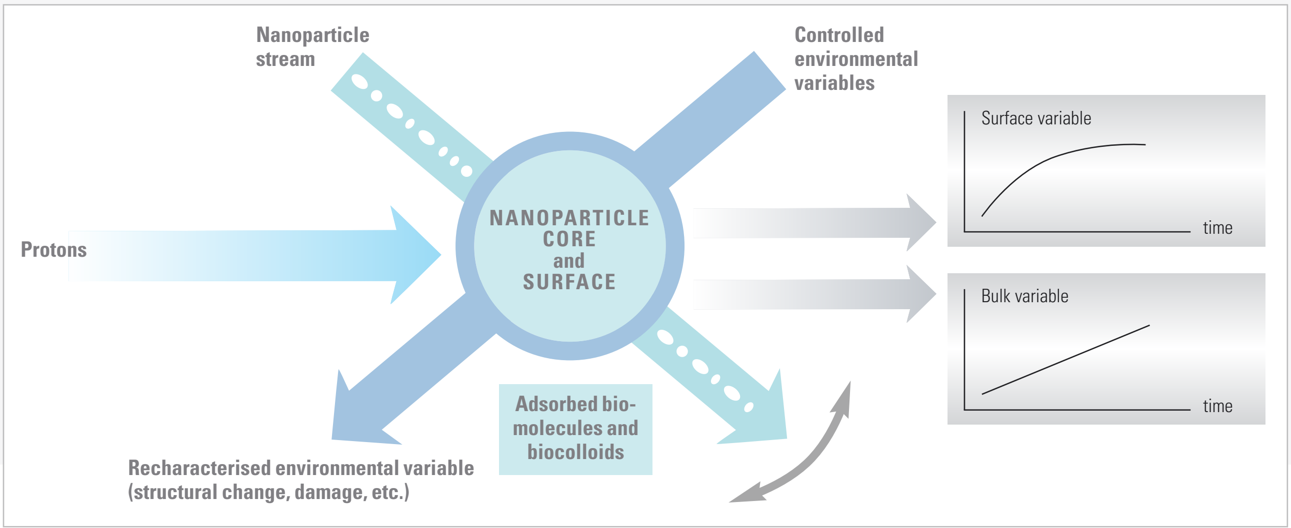


Fig. 11.6.5: Nanoparticle processing and monitoring pathways for controlled ageing and biosample exposure.

ciation, hydration, size distribution), but through controlled environmental exposure, a critical assessment of changes in these baseline parameters in specific aqueous biometrics. The latter affect, surface oxidation, corrosion, bulk hydration, degradation and dielectric properties are operationally quite different inside and outside of the cell. This 'aging' phenomenon is poorly understood, and has been difficult to study using normal analytical tools. Adaptation of SAXS and neutron scattering to the dynamics of nanoparticle interactions in the aqueous phase would enable rational nanoparticle design as well as ensure reproducibility and standardisation as a basis for regulatory approval.

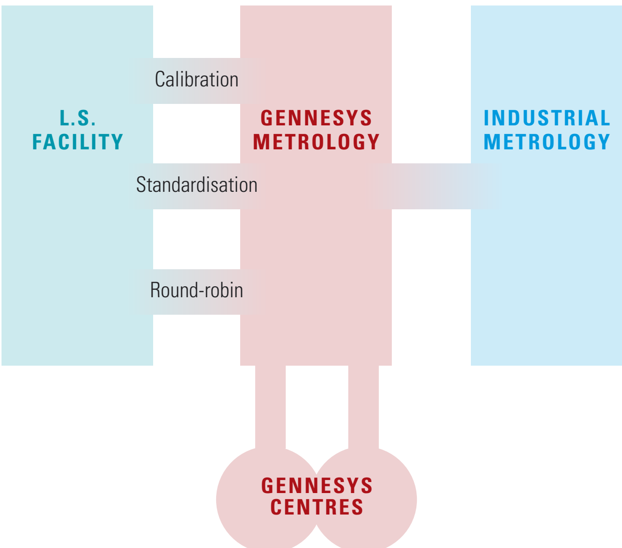


Fig. 11.6.6: Place of GENNESYS in the nanostandardisation scheme.

11.6.3. ORGANISATIONAL SCHEMES FOR NANO-STANDARDISATION WORK AT LARGE-SCALE FACILITIES

GENNESYS-metrology should play an interface role between the metrology research laboratories, industry and the large-scale facilities in order to incorporate synchrotron radiation and neutron techniques in nanomaterials and manufacturing processes (see Fig.11.6.6). In addition, it should be tightly connected to the GENNESYS science and technology centres. Neutrons and synchrotron facilities offer specific techniques using sources which are different from the sources available in industry/metrology laboratories. It is therefore essential to extend the usual metrology activities to the measurements carried out at large-scale facilities. GENNESYS-metrology will have to develop calibration, standardisation and round-robins in order to match the requirements of companies.

11.6.4. CONCLUSIONS AND RECOMMENDATIONS

The absence of central facilities for full parameter characterisation of nanoparticles/materials is a bottleneck to advances in this critically important field; it is strongly encouraged to create a GENNESYS Centre of Excellence in nanostandardisation and nanometrology. This would provide a scientific- and industrial infrastructure in Europe for dimensional nanometrology and nanostandards specification (nanochemical, nanomechanical, nanobioproperties, nanoelectronics etc.), reference materials and standard measuring methods.

In addition, this European centre would also become the European meeting point for European/international standardisation and metrology for nanomaterials using synchrotron radiation and neutron techniques.

11.7. KEY CHALLENGES FOR INDUSTRY

Within the last 10 years, nano-structured materials have emerged as a key field: they offer a large spectrum of most interesting properties (see Fig. 11.7.1).

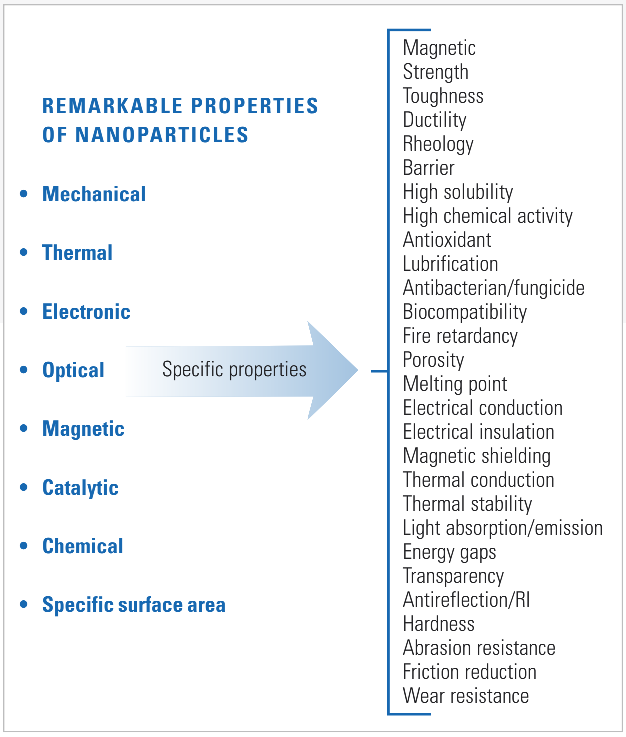


Fig. 11.7.1: Properties of nanoparticles.

The applications are enormous: ranging from informatics and communication over bio-nanosystems, energy and so on (see Fig. 11.7.2). The scale of the nanostructures typically ranges from fine structured industrial materials, with sizes in the sub-microns, to completely new materials with dimensions of tens of nanometres. The research field therefore combines basic and applied research with both near time and future applications in society (see Fig. 11.7.3).

European nanotechnology industry needs the utmost research tools

- To remain competitive the industrial companies are more and more obliged to innovate and to use the most powerful tools for their research, development and quality control activities;
- Understanding and controlling the behavior and the manufacture of nanomaterials represents today a technological and scientific challenge that the European industry must raise successfully to position in a competing way compared to North-American industry or of the South-East Asia;
- This is particularly crucial for the field of the nanotechnologies which exploits new properties of materials based on their behavior on a scale which still remains to be explored and for which the usual tools of modeling are not well adapted.

European large-scale facilities try to open up to applied activities

- The large-scale facilities offer unequalled possibilities for material analysis, in particular the synchrotrons and neutrons facilities. These platforms were initially designed as tools for research fundamental with, as unique evaluation criterion, the quality of the scientific publications of their users.

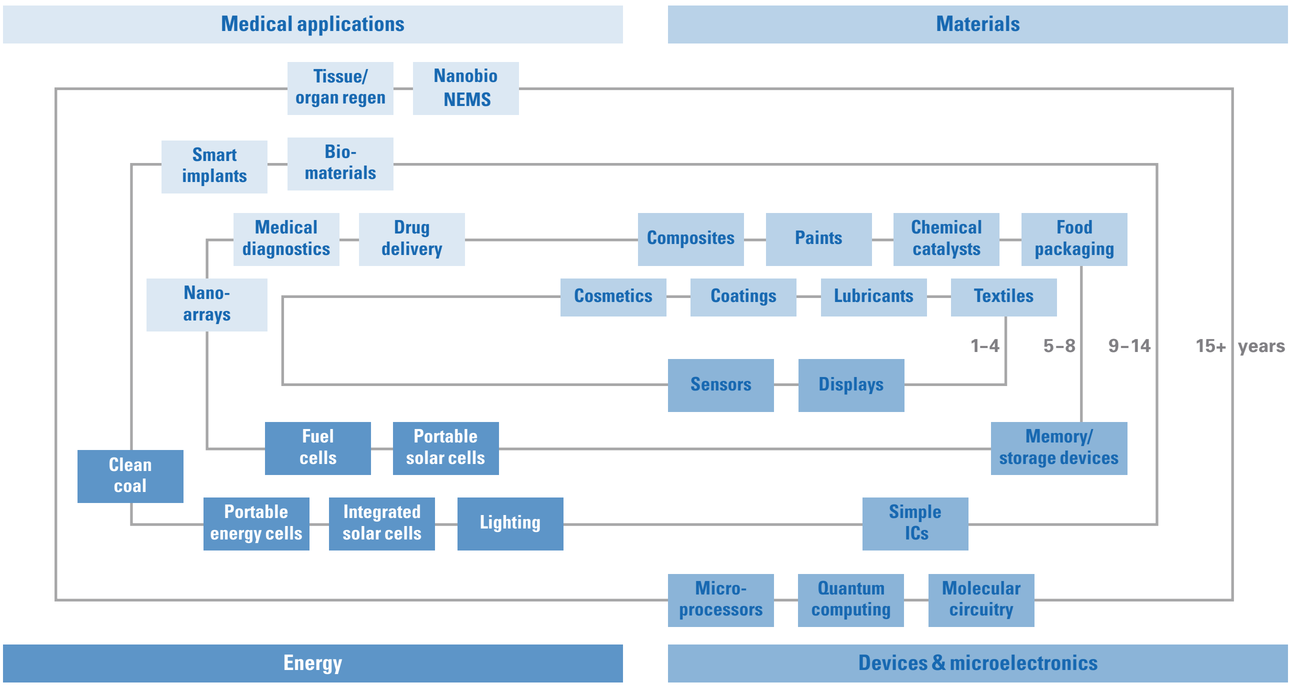


Fig. 11.7.2: Key highlights for nanomaterials applications in industry.

- Conscious to have now reached a stage of performances and reliability compatible with a use by the industrialists, and gain notoriety, the large-scale facilities now wish to invest towards the applied activities.
- Industry needs a fast and cheap access to the techniques; most of the time, long delays are requested and the expertise is not available in the company, requiring scientific- and technical assistance from the large test facilities;
- However, their culture and their operating process do not facilitate this opening which remains still too limited today in regard to the importance of the challenge for European industry.

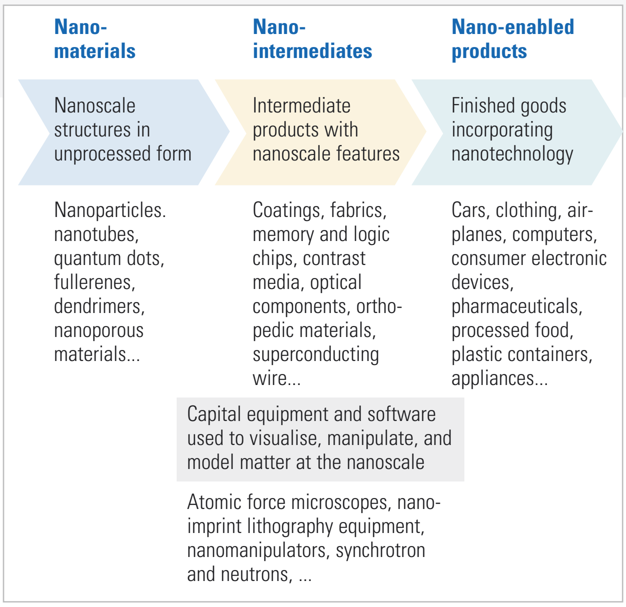


Fig. 11.7.3: Nanomaterials applications in industry and the value chain.

GENNESYS-Industry to bridge the gap between European industry and large scale research facilities (Fig. 11.7.4)

- The finding is therefore clear. On the one hand there is the European nanotechnology industry that needs to put all the strengths of his side to benefit from the best scientific data on materials it develops, on the other hand large facilities can provide such data but are not yet adapted to the industrial use despite their efforts.

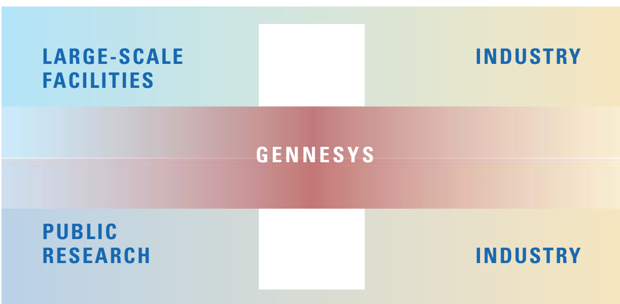


Fig. 11.7.4: GENNESYS and the bridge between industry and large-scale research facilities.

- Hence the need to create an interface structure, GENNESYS-Industry, whose mission is to bridge the gap between nanotechnology companies and large scientific facilities.

The missions of GENNESYS-Industry

- GENNESYS-Industry will not only boost the interface between enterprises and large scientific facilities but also interact with all the actors who have scientific expertise, firstly university laboratories.
- As company researchers don't understand what the benefits from the large scientific test facilities techniques are. An important mission of GENNESYS-Industry will consist in advertising companies i.e. through "success" stories.
- The management of GENNESYS-Industry will follow a bottom-up approach, seeking to implement the recommendations made by industrialists from various strategic and thematic committees to be established.
- Nearby large-scale facilities, several platforms GENNESYS-Industry will be developed around large scientific facilities.
- GENNESYS-Industry will seek to develop "pocket" facilities in order to democratise their use by making it accessible when it can not be practised on site, for example, control activities of production or treatment in hospital.

The GENNESYS-Industry technical platforms

Each GENNESYS-Industry platform, focused around an urgent topic, will be designed

- to update industry on new analytical and technological possibilities available to them at neutron and accelerator-based x-ray facilities;
- to assess the scientific and technical needs of industry;
- to adapt/upgrade the analytical equipment to the needs and constraints of industry;
- to assist the industrialists or take charge of their analyses;
- to accommodate industrial teams with new projects;
- to acquire and manage a fleet of instruments;
- to assure rapid access to dedicated analytical techniques for industrial partners for urgent check of the performance of new concepts and processes and potential failure mechanisms in new devices and nano-architectures;
- to guarantee the confidentiality of data;
- to contribute to a responsible partnering between academia and industry in a new world of open innovation.

The technology platform will host research teams over periods of several days to several years to work on projects involving the use of the analytical portfolio developed by GENNESYS personnel (including its own standardised beam line/s).

GENNESYS-Industry will benefit industries from all Europe

- GENNESYS-Industry, with its various technical platforms, will enable industrialists from countries who do not operate any large-scale facilities, in particular those from Central and Eastern Europe, to benefit more easily of these exceptional analytical tools.
- Today, for geographical reasons, it is mainly companies from Western

countries who use these facilities. Open platforms to all European countries will help increase business performance regardless of their location.

- GENNESYS-Industry will also contribute to boosting technology transfer between large scale facilities and European industry and will rise to the creation of numerous spin-off companies.

GENNESYS-Industry involves the active contribution of several partners. Its success will depend on a good co-ordination between the tasks attributed to each partner:

- the industrial companies will define their analytical needs;
- the large scale facilities will provide the necessary analytical technology and appropriate access;
- the academic laboratories will contribute relevant scientific expertise;
- the national funding agencies will support the activities of GENNESYS-Industry and its platforms.

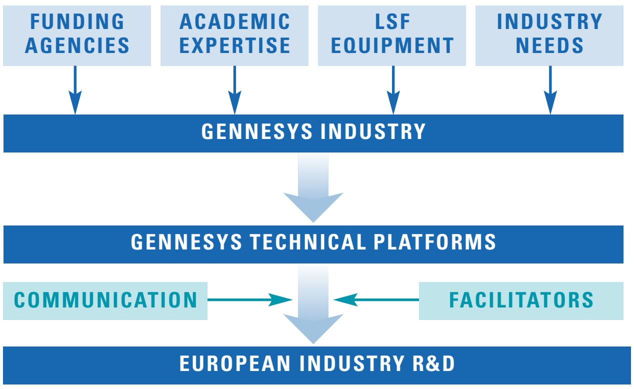


Fig. 11.7.5: The organisation of GENNESYS – Industry I.

By this joint effort, the four partners will enable the creation and sustainable successful operation of GENNESYS-Industry.

The organisation of GENNESYS-Industry relation (Fig. 11.7.5)
In order to encourage and foster the transfers of scientific breakthroughs in nanotechnology to industry ("open innovation scheme), the GENNESYS-Industry platform should create a responsible partnering and fruitful climate for entrepreneurship and business developments. To do so the dialog and interaction within the triangle industry (SMEs's and global players), large scale research facilities as well as universities has to be strengthened considerably. Both top-down and bottom-up measures are necessary.

Top-down scheme (Fig. 11.7.6)
An advisory board of highly ranked research managers from industry, including providers of venture capital, directors of large-scale facilities and presidents of the leading European Research Universities, should be established.

This board defines/upgrades/revises, on a regular basis (typically during an annual meeting), specific research topics in nanotechnology research; direct and efficient transfer to industry being the most urgent topics. These topics will be pre-discussed within expert groups which meet regularly and report to the advisory committee. Industry and providers of venture capital will use this board as a platform to identify strong and suitable research partners and new trends in nanotechnology and corresponding products. Facility and university managers have the possibility to identify the specific research needs of a global industry at a very early stage.

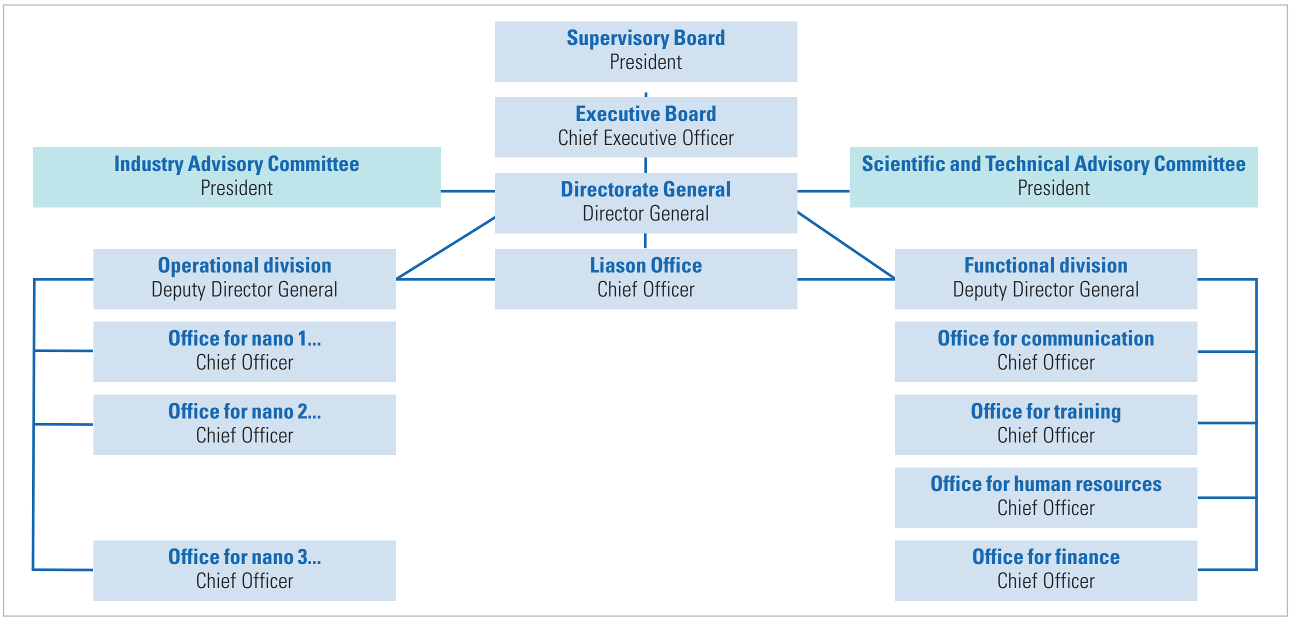


Fig. 11.7.6: The organisation of GENNESYS – Industry II.

Bottom-up scheme

These working groups bring together the experts from industry, large-scale facilities and universities. They are the essential platform for the bottom-up approach. It provides a venue for researchers to meet developers of high-tech nanotechnological products. These platforms, workshops and discussion forums have to present precise ideas and potential first applications of the specific nanotechnology to the advisory board.

Measures

To leverage better interaction between the three partners, several measures are proposed:

- Industry has to participate in the advisory committees of universities and large scale facilities.
- Large-scale facilities need trained personal devoted to address the specific needs of industrial and commercial research partners..
- Entrepreneurial attitudes have to become a part of the scientific culture at large scale facilities. Specific training/education may be needed.
- Industry and academia have to quickly adjust to the new world of open innovation which requires the underpinning of a sustainable future technology by a robust data base.
- Large-scale facilities have to establish quality assurance for their industrial products and processes. This quality assurance has to be standardised among several large scale facilities.

Conclusion

Innovation in new technologies is mandatory to keep European industry at the forefront of worldwide competitiveness. Nanotechnologies offer today for all industrial sectors the largest capabilities for developing innovative products with new functionalities. The "nano" revolution is based on the properties of materials at a new length scale which are far from being explored. To investigate and understand this novel scale and exploit efficiently and rapidly the enormous potential of nanosciences for applications it is necessary to strengthen the links between academic research and industrial activities. This must be done primarily by offering to the European industry an application-oriented access to the large scientific infrastructures (mainly synchrotron and neutrons large-scale facilities) to benefit from the utmost analytical and characterisation tools and therefore to speed up the development of nanobased products. A great effort should therefore be made to transform and open the large European facilities, which are basic research-oriented, to industrial use for research, development, control of quality and recycling.

The mission of GENNESYS-Industry is:

- to bridge the gap between the European research infrastructure and high tech companies;
- to advertise companies of these new possibilities and to train their engineers;
- to mitigate current difficulties in knowledge transfer between academia and industry.

GENNESYS-Industry will promote a responsible partnering between academia and industry creating a synergetic research environment beneficial for all partners and for the society. GENNESYS aims to strengthen the collaboration between universities and large scale facilities for the purpose of advancing nanotechnology and finally to enable the efficient transfer of this technology to industry. In order to capitalise on the fragmented intellectual potential at research institutions and industry, a number of necessary key actions have been identified (see Fig. 11.7.7).

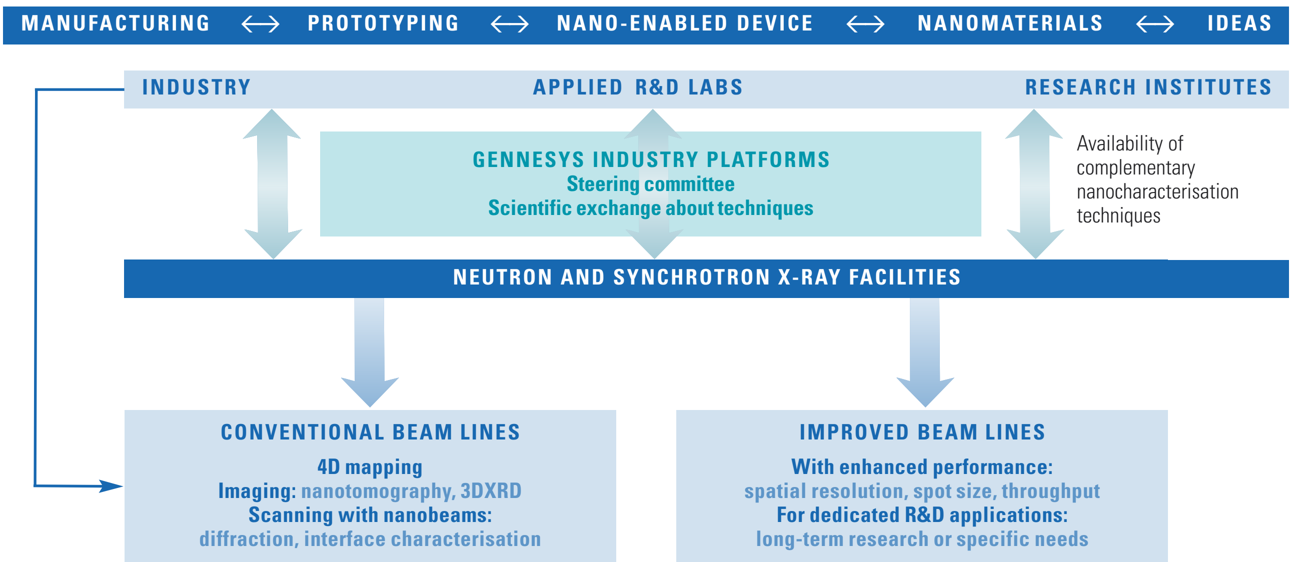


Fig. 11.7.7: GENNESYS Industry Platform

11.8. KEY CHALLENGES FOR LARGE-SCALE RESEARCH FACILITIES

Nanoscience and nanotechnology have become the future challenge for materials scientists, policy-makers and forward-looking industries. The breakthroughs in this field offer new opportunities for all key technologies, encompassing health and medicine, electronics, information technology and manufacturing, energy, environment and climate change. The European research infrastructure must play a key role in Europe´s future strategy for the development of novel nanomaterials with outstanding properties and performance. This research strategy is an interdisciplinary effort which involves universities, research laboratories and industry and requires that top-class fundamental as well applied research in materials science is supported at Europe's large-scale facilities, i.e. synchrotron radiation, laser and neutron sources. Today, basic research in nanoscience is still too much fragmented across the EU and not coordinated in a strategic way to solve the urgent problems of today and tomorrow.

Synchrotron radiation and x-ray laser facilities*	Location	Electron energy (GeV)	Number of beam lines
ALBA (1st phase)	Spain	3	7
ANKA	Germany	2,5	15
BESSY	Germany	1,8	21
DIAMOND	UK	3	27
DORIS III	Germany	4,5	20
ELLETRA	Italy	2,2	26
ESRF	EU (France)	6	32
European XFEL Hard x-ray laser 1st Phase in construction, start 2013	EU (Germany)	20	3–5
FELBE IR Laser	Germany	0,04	2
FLASH Soft x-ray laser	Germany	0,45	3
ASTRID II	Denmark	1,4	
MAX IV in construction, start 2009	Sweden	1,5/3	14
PETRA-III in construction, start 2010	Germany	10	14
SLS	Switzerland	2,4	17
SOLEIL	France	2,75	
SRS closing 2008	UK	2	11

Neutron facilities*	Location	Thermal power	Number of beam lines
BENSC	Germany	10	32
BNC	Hungary	10	10
FRM-II	Germany	20	27
ILL	EU (France)	58	34
ISIS Spallation source	UK	–	26
JEEP-II	Norway	18–25	??
LLB	France	14	23
RID	Netherlands	2	3–4
SINQ Spallation source	Switzerland	–	19
FRG-1 closing 2009	Germany	5	
*(alphabetic order)			

Table 11.8.1: List of European synchrotron radiation and neutron facilities.

Through the GENNESYS initiative, a European consortium of institutes, universities, and neutron and accelerator-based x-ray facilities, has been is working to bridge the gap between the research needs and future challenges of the nanotechnology community, and matching this with the revolutionary analytical developments at neutron and synchrotron radiation and laser facilities. In order to stay competitive at the international level, Europe has to make the best use of its highly developed network of large-scale facilities (see Table 11.8.1), this in turn implies also matching beam line specification, operation of and access to these facilities to the needs of public and private research institutions.

The GENNESYS initiative has brought to light that the future analytical barriers for the development of nanomaterials for new technologies can only be overcome, if the demands of nanomaterials science and the analytical potential of synchrotron radiation and neutron sources are brought together for new breakthroughs in nanomaterials synthesis, functions and modelling.

Synchrotron and neutron facilities in Europe are dedicated to providing the best possible interdisciplinary research infrastructure for all scientists. They are under continuous development, and of at the forefront of analytical technologies. Both types of facilities have achieved a range of excellent techniques for nanoscience and nanotechnology, in particular in the range of non-destructive characterisation and in-situ monitoring and testing. Today, advanced accelerator-based x-ray and neutron techniques, as provided by the modern European facilities, are applied to challenging problems in physics, chemistry, medicine, in biological science, as well as in environmental and engineering sciences, geological, archaeological science and cultural heritage. These highly sophisticated techniques are highly relevant for the development of tailored nanomaterials needed for current and future urgent problems of our society.

Building on the inherent strength of the technique, neutron facilities profit from new technologies which upgrade the performance of their resources and instruments. The upgrade of these facilities is driven by the users who require more sophisticated experiments on cutting-edge science and will focus on improved flux and higher resolution (both in space and time) which allow increasingly precise measurements on increasingly smaller (0.001 mm^3) or more dilute (10 ppm) samples, and faster kinetic studies. Clever use of the neutron spin will most likely lead to novel ways to interrogate buried nanostructures with a high level of precision. The efficient interplay of the neutron facilities and untrained users is essential for success. There are already working examples of such collaborations in several scientific areas including engineering and biology. However, regarding nanomaterials research as defined by the GENNESYS scope, a more powerful European neutron facility ("European spallation source") has to be envisaged together with the full integration of support laboratories and facilities. Dedicated sample environments and even complete spectrometers, as well as on-site expertise, are required to exploit the full potential of this powerful technique. In addition, in-situ integration with other experimental probes, such as differential scanning calorimetry, x-rays or optical spectroscopy, is also called for.

Synchrotron radiation has developed in a truly revolutionary manner during the last decades. In order to become internationally competitive in nanoscience, European synchrotron radiation sources need to be optimised for high brilliance and stability and for the special needs of the nanomaterials science community. For the application of synchrotron radiation to future challenges in nanomaterials development, novel beam lines have to be devised and x-ray optics and x-ray detectors have to be improved. X-ray optics is currently limited by technology. Major technological developments are needed in metrology and nanofabrication in order to improve their performance, both in terms of efficiency and imaging quality. In addition, fundamental research in x-ray optics is needed to probe the physical limits of x-ray microscopy. Fast and massively parallel detectors optimised for detection quantum efficiency, spatial resolution, and dynamic range are needed, in particular in view of nanoscience applications at x-ray free-electron lasers.

Thus, a concerted effort at the European level is required to dedicate and optimise synchrotron radiation beam lines for nanoscience applications. This includes optimisation of the beam lines for optimum performance, improvement of the stability of all beam line components, and high precision mechanics. In order to make optimal use of x-ray microscopy, special sample environments for in-situ studies compatible with nanoprobe techniques are needed, such as high pressure cells, miniature chemical reactors (microfluidics), cryostats, ovens, or magnets.

Significant improvements over synchrotron radiation sources in terms of brilliance and time structure are expected from free electron lasers and energy recovery linacs (ERLs). The XFEL will offer unique opportunities for nanomaterials science, especially for non-crystalline matter and time-resolved studies in the femtosecond domain. In order to make optimal use of this facility, a lot of basic instrumental and methodological developments will have to be done. This conclusion is strongly supported by the experience gained at the FLASH facility.

Key techniques and requirements that need to be developed to a high standard and made available for nanomaterials users are:

- High-resolution beams down to 10–20 nm size at synchrotron radiation and laser facilities and down to <100 microns at neutron facilities, for the study of nanostructures, thin films and coatings;
- Full 3-D reconstruction of nanostructures;
- Combination of scattering, imaging, and spectroscopy on the same sample spot;
- Scattering techniques with magnetic sensitivity;
- X-ray imaging techniques under relevant environments;
- X/n tomography for nanomaterials under relevant environments;
- Time-resolved diffraction techniques which allow following dynamic processes like domain wall propagation, diffusion, spin precession, surface formation/transformation, chemical reactions in real-time;
- In-situ nanomaterials manipulation and processing capabilities;
- Real-time multi-scale monitoring of materials fabrication, industrial processing and nanostructure development;
- Neutron and synchrotron instrumentation capable of studying nanodevices & components operated under realistic conditions (see Fig. 11.8.1);
- Dedicated beam lines with sufficient physical space to house prototype process plants, large engineering samples and sample manipulation devices;
- Faster experiment turn-around at facilities to accelerate product development with industrial and academic involvement;
- More efficient collaboration between facilities, academics and industrial teams in designing/carrying out experiments – this would be aided by a pioneering Structural Nanomaterials Centre (see Fig. 11.8.3), providing leadership and unique nanomaterials processing and handling facilities;
- Improved software tools for experimental planning, design, implementation and data analysis, so that a greater proportion of beam time is used in obtaining useful data;
- Education of materials engineers with experience in neutron and synchrotron diffraction techniques;
- Better links between basic research, materials characterisation, materials engineers and end users.

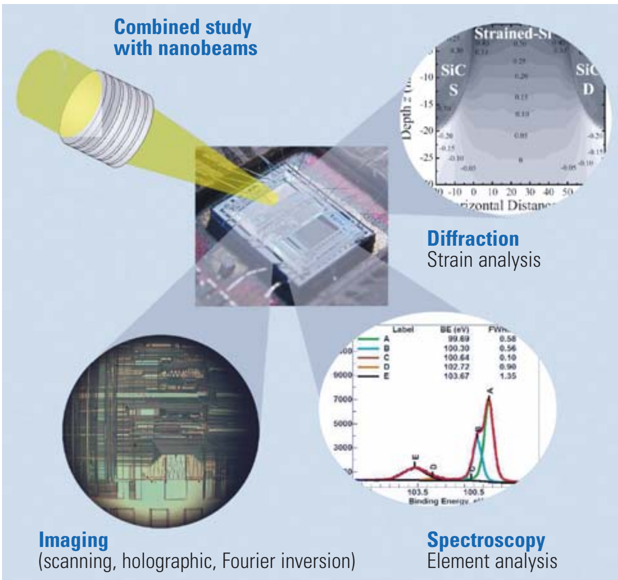


Fig. 11.8.1: Nanobeam analysis for improved device performance (example).

GENNESYS is at a crossroads for the integration of nanomaterials science at a European level. From a facilities point of view, the establishment of the following facilities through GENNESYS are key to ensuring future breakthroughs in the development of novel nanomaterials:

- **Dedicated User Support Facilities (USF)**
  It is mandatory that high-tech USF's be created in close neighbourhood to synchrotron radiation, laser and neutron facilities for the preparation and handling of delicate samples, as well as for the performance, analysis, interpretation and evaluation of an experiment. These USFs are a major upgrade of the current "local contact" practice of the large-scale facilities, as they should provide a critical mass of the necessary basic technology and knowledge support for the:
  - User groups, particularly of the untrained users from all nanomaterials research sectors;
  - GENNESYS Science and Technology Centres on site (see below).

The scientists and engineers of the USF's should establish contact with the users sufficiently prior to the experiment for optimising the experimental conditions, during the experiment for guaranteeing a successful data harvesting and after the experiment for assuring maximum output. The scientists and engineers of the USF's should also participate in the regular training courses (see below).

USF's will include nanosynthesis, micro- and nanomanipulation and pre-characterisation of delicate samples as well as proper software and instrument control methods in such a way that the operation of dedicated instruments for nanosciences is made routine and for high-throughput, allowing nanomaterials scientists to make the best use of large-scale facilities in order to obtain fast and reliable answers to their engineering problems. USF's will develop specialised sample environments for in-situ studies of nanomaterials, i.e. ambient conditions, high-pressure, high-temperature, controlled humidities, controlled chemical environments, high magnetic and electric fields, external mechanical loads.

In order to develop the full potential of the USF's, a strong and sustainable in-house research programme in nanomaterials science should be built up at the associated large-scale facilities.

- **"From open access to strategic access"** (Fig. 11.8.2)
  Until today, the European large-scale facilities for the fine analysis of matter have been operated exclusively in the "open access" mode (OAM) based on a transparent peer review system assuring scientific excellence. In this way, these facilities leveraged the clever ideas from research groups of all sectors. The research profile of OAM facilities is thus largely determined by the scientific visions of the external users.

  The strategic development of tailored nanomaterials for urgent technologies requires a paradigm change in the operation of the European research infrastructure:
  - The dedication of a fraction of the available analytical technology to strategic research;
  - Access and to upgrade it to the specific needs of the GENNESYS consortium.

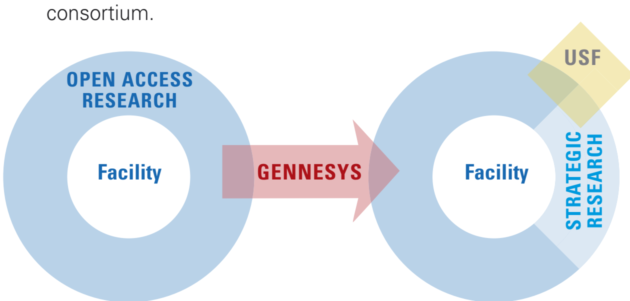


Fig. 11.8.2: GENNESYS recommendation for strategic access.

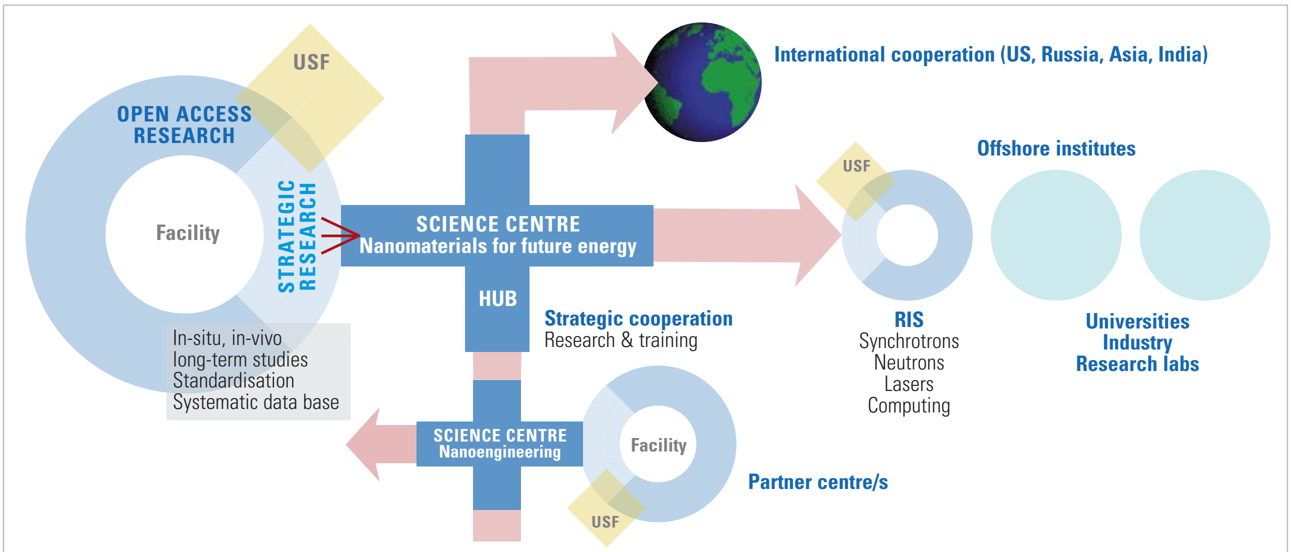


Fig. 11.8.3: Science Centres and the European integration in nanomaterials research.

This partial transformation of a European facility into a strategic operation is prerequisite to allocate a GENNESYS Science and Technology Centre and/or to be member of a European research platform.

- **GENNESYS Science and Technology Centres** (see Chapter 11.11)

The strategic knowledge-based development of new nanomaterials which are needed to solve urgent problems of society require the creation of GENNESYS Science Centres which cooperate in a new way with the European research infrastructure. GENNESYS strongly recommends that these Science Centres which focus onto urgent topics in nanomaterials development are built in direct contact with neutron and accelerator-based x-ray facilities. The structure and organisation of these new centres are described in Chapter 11.11. They are building hubs for research and training and exploit the strategic part of the analytical portfolio of the associated large-scale facility for:

- In-situ monitoring of nanoparticle synthesis;
- Long-term studies of nanomaterials and device performance;
- Systematic and combinatorial investigations of complex nanomaterials architectures;
- Direct and immediate access to diffraction, spectroscopy, imaging, tomography of sensible and nanostructures;
- Standardised nanocharacterisation;
- Long-term studies of degradation and failure;
- Building up a data base;
- GENNESYS Training Centres.

The future scientific and technological challenges associated with the development of nanomaterials require a new generation of scientists with an interdisciplinary research background. Since the design of nanomaterials is the paradigm for an interdisciplinary research effort merging the traditional fields of physics, chemistry, engineering and biology, the appropriate education of young scientists is a big concern. In order to cope with the barriers, one needs experts in particular fields and "not shallow water scientists" who understand a little of everything. To offer the proper education scheme which produces top-notch experts who simultaneously have the necessary literacy in neighbouring fields, must be the goal of European Training Centres. The GENNESYS infrastructure must be exploited to provide such a training and education platform. By collaboration with universities and industry and by providing direct access to large-scale experimental set-ups, including the integrated User Support Labs, the GENNESYS Science Centres should become core partners is such a European effort. Among the future tasks of GENNESYS Training Centres are:

- Partner institutes for new interdisciplinary education schemes for young scientists (see Chapter 11.9);
- Training of scientists from PhD level in the use and methods of nanofunctional materials science;
- Creation of awareness of capabilities also in the engineer and management level;
- Transfer of knowledge to companies through educated scientists and engineers.

By following the GENNESYS roadmap, the existing European research infrastructure will contribute in a strategic way to a sustainable growth by underpinning the development of new technologies with pre-competitive R&D and with the database on a nanoscopic level. In tomorrow's world which will be determined by the new paradigm of "open innovation", breakthroughs in all key technologies require the intimate handshake between fundamental research in nanoscience and industry.

This new strategic role of the European infrastructure for fine analysis will underpin (Fig. 11.8.4):

- The development of new materials for energy production and more efficient energy use as well as energy saving;
- Minimising environmental impact due to improved fabrication methods ("green technology"), improved monitoring systems;
- Improvements in health care and medical diagnostics;
- The progress of new IT technologies;
- The security and surveillance systems.

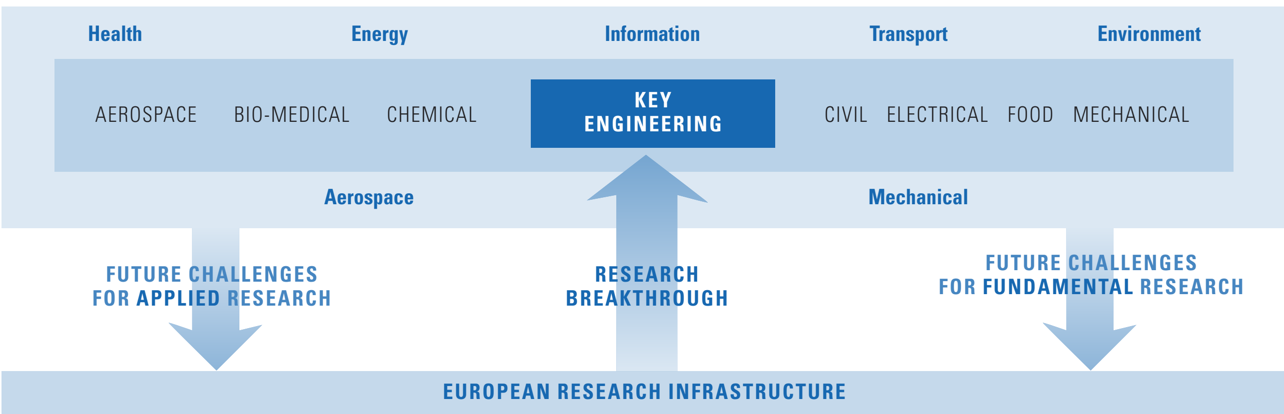


Fig. 11.8.4: Diagramme showing how the European research infrastructure is integrated in an "open innovation" scheme.

11.9. KEY CHALLENGES FOR EDUCATION

In order to face up to the massively sectorial investments of major or emerging countries targeting world leadership in some economic areas, Europe and partner institutions must overcome the fragmentation of the human and materials resources of European Research. This can be done by gathering the best teams to share these resources through integrating them into new European organisations (GENNESYS European College of Excellence). The GENNESYS initiative represents a unique and attractive opportunity to gather and integrate geographically dispersed human resources and effectively scientific facilities for training and promoting activities (see Fig. 11.9.1).

Many companies throughout Europe and the world report problems in recruiting the types of graduates they need, as many graduates lack the skills to work in a modern economy. For Europe to continue to compete alongside prestigious international institutions and programmes on nanomaterials, it is important to create a "Europe Elite College" which provides a top-level education and the relevant skills mix. This should be a new institution, involving new "satellites" of leading universities and other institutions throughout Europe. Such a college should cover education, training, sciences and technologies for research, and have strong involvement by European industry.

The elements for such a high level education are:

- Multidisciplinary skills;
- Top expertise in nanomaterials science & engineering;
- Literacy in complementary fields;
- Exposure to advanced research projects;
- Literacy in key technological aspects: exposure to real technological problems;
- Basic knowledge in: social sciences, management, ethics, foreign languages;
- Literacy in neighbouring disciplines: International business, law, etc;
- Interlinkages between: education, research and industrial innovation: students will be ready for that research and development will provide;
- Sharing of post-docs, Masters and PhD students to foster the mobility of permanent researchers and professors between different institutions are needed to create "team spirit".

The new European College for Nanoscience will offer both education and training. The training will cover master's degrees and professional doctorates, linking university researchers and training for industrialists with recognised qualifications. The European College should have strong links with universities of excellence in Europe, nanomaterials research institutes, the research infrastructure and industry. The GENNESYS Centres of Excellence should play an important role.

A European action plan in nanomaterials education has to be worked out urgently to underpin a sustainable nanomaterials research strategy. Strong efforts must be undertaken to improve integration of nanomaterials education and research, particularly at the boundaries of disciplines and to prepare flexible and adaptable nanomaterials scientists and engineers for the future.
A new framework of cooperation between universities, national research institutes and industry needs to be developed.

The proposed GENNESYS Nanomaterials European College would ideally meet the requirements for the training of our future materials scientists and engineers. It would be a central institute with satellite schools at the GENNESYS "Centres of Excellence"– and with close associations to recognised research universities and corporate research in industry throughout Europe.

GENNESYS International Institute for Nanomaterials is ideally complementing the EIT (European institute for Innovation and Technology). Joining both institutions would become the motor for "Innovative Europe" in nanomaterials science and technology.

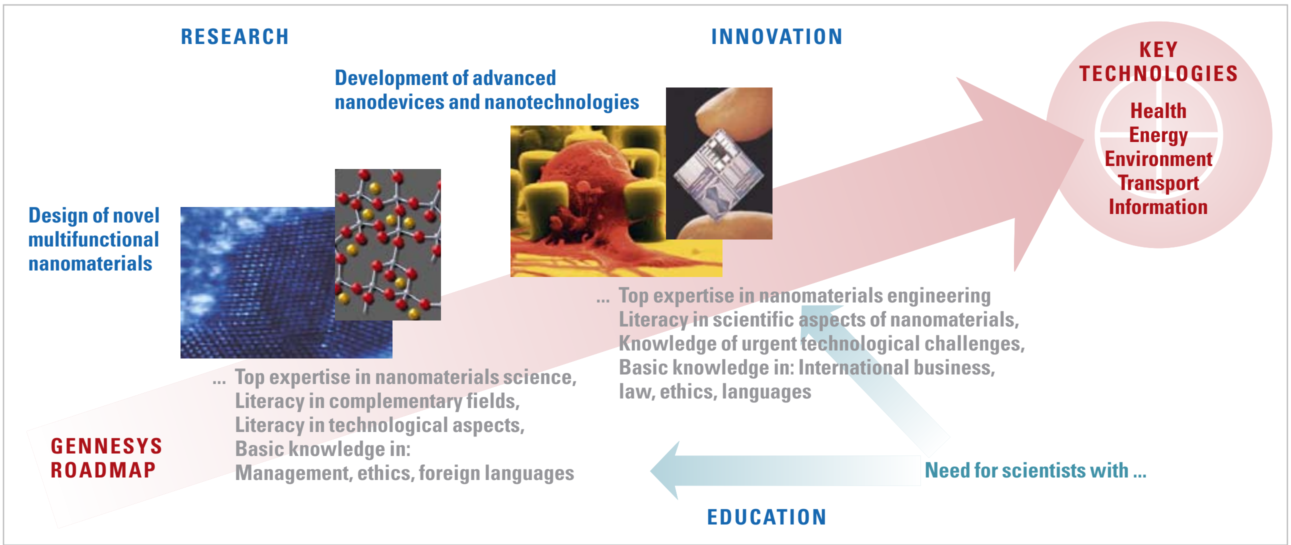


Fig 11.9.1: The education challenge in nanomaterials science and technology.

11.10. KEY CHALLENGES FOR NANOMATERIAL SCIENCE AND SOCIETY

The impact of nanotechnologies will be accompanied by changes in the social, economical, ethical and ecological spheres. The further development of nanotechnologies will be dependent upon the consumer's acceptance of nanomaterials and nanotechnology-enabled devices, the ethical and social, health and safety implications of nanotechnology, and lastly, the environmental impact of nanomaterials. Consequently, it is prerequisite to: educate the public, assess and manage the potential risks associated to the development of nanotechnology, and to accurately disseminate nanotechnology development results in an open way so that the general public's acceptance of nanotechnology can be gained. European synchrotron radiation and neutron facilities should contribute to the public awareness of nanoscience and nanotechnology by:

- Educating the public about the benefits and potential risks of nanomaterials and nanosystems;
- Evaluating, minimising and even eliminating the risks associated with the manufacturing, use and disposal of nanomaterials and nano-enabled products.

• Social benefits of micro- and nanotechnologies

Today, the daily use of high-tech materials and devices from micro- und nanotechnologies has become widespread. In the near future, the development of nanotechnology will lead to a wide range of consumer products with improved performance, a longer lifetime and lower costs, and within which the use of nanomaterials will be effectively 'hidden' from the end user. New medical treatments and potential disease cures will be based on nanotechnologies.

The benefits will be present across all industrial sectors and throughout the full spectrum of consumer applications:

Consumer electronics

- Low power consumption and low cost microprocessor and memories;
- Low voltage displays and televisions with enhanced resolution and significant reduced purchase and operating costs;
- High density magnetic data storage thanks to the use of spintronics and nanowires;
- High sensitivity and wireless sensors for detecting various parameters such as electrical resistivity, chemical activity, thermal conductivity, and tire pressure.

Energy production and storage

- High energy density batteries with higher capacity and better cycle lifetime;
- Large and low-cost photovoltaic solar cells.

Medicine and healthcare

- Smart drug delivery;
- Laboratories-on-a-chip for personalised drug development and molecular diagnostics, such as safe and timely bio-detection to avoid pandemics;
- Antimicrobial nanopowder and coatings;
- Cancer diagnosis, accurate tumour location;
- Gene transfection and therapy;
- Nucleic acid sequence and protein detection.

Environmental applications

- Elimination of pollutants;
- Self-cleaning windows;
- Water remediation;
- Conservation of resources;
- CO_2 and aerosol emission reduction.

• Societal acceptance of micro- and nanotechnology

One central question about the development of nanotechnology is whether the unknown risks of engineering nanoparticles and nanotechnology-enabled products, in particular their health and environment impact, outweigh their established benefits. The lack of reliable and accurate technical data on the topic provides fertile ground for both nanotechnology proponents and sceptics to make contradictory and sweeping conclusions about the safety of engineered particles and products based on them.

It is imperative to carry out investigations devoted to the development of a comprehensive understanding of the properties, interaction, and fate of natural and anthropogenic nanoscale and nanoengineered materials in the human body and environment. Necessary research activities are:

- Developing strategies for safe manufacturing, use and disposal of nanomaterials;
- Understanding how the morphology, size, composition, surface reactivity, agglomeration, kinetics and transport of nanoparticles (nanotoxicity) affect human health and environment, including climate change;
- Investigating the kinetics and biochemical interactions of nanoparticles with organisms;
- Studying nanoparticle aging: surface modifications and change in aggregation state after interaction with bystander substances in the environment and with biomolecules and other chemicals in the organisms.

Developing robust ways of evaluating the potential impact – good or bad – of a nanotechnology-enabled product from its initial manufacture and use to its ultimate disposal, which must engage both scientific and policy communities (Fig. 11.10.1).

Communicating research results on the assessment, minimisation and prevention of nanotechnology risks and benefits outside the scientific community is challenging, but it is essential for its develop-

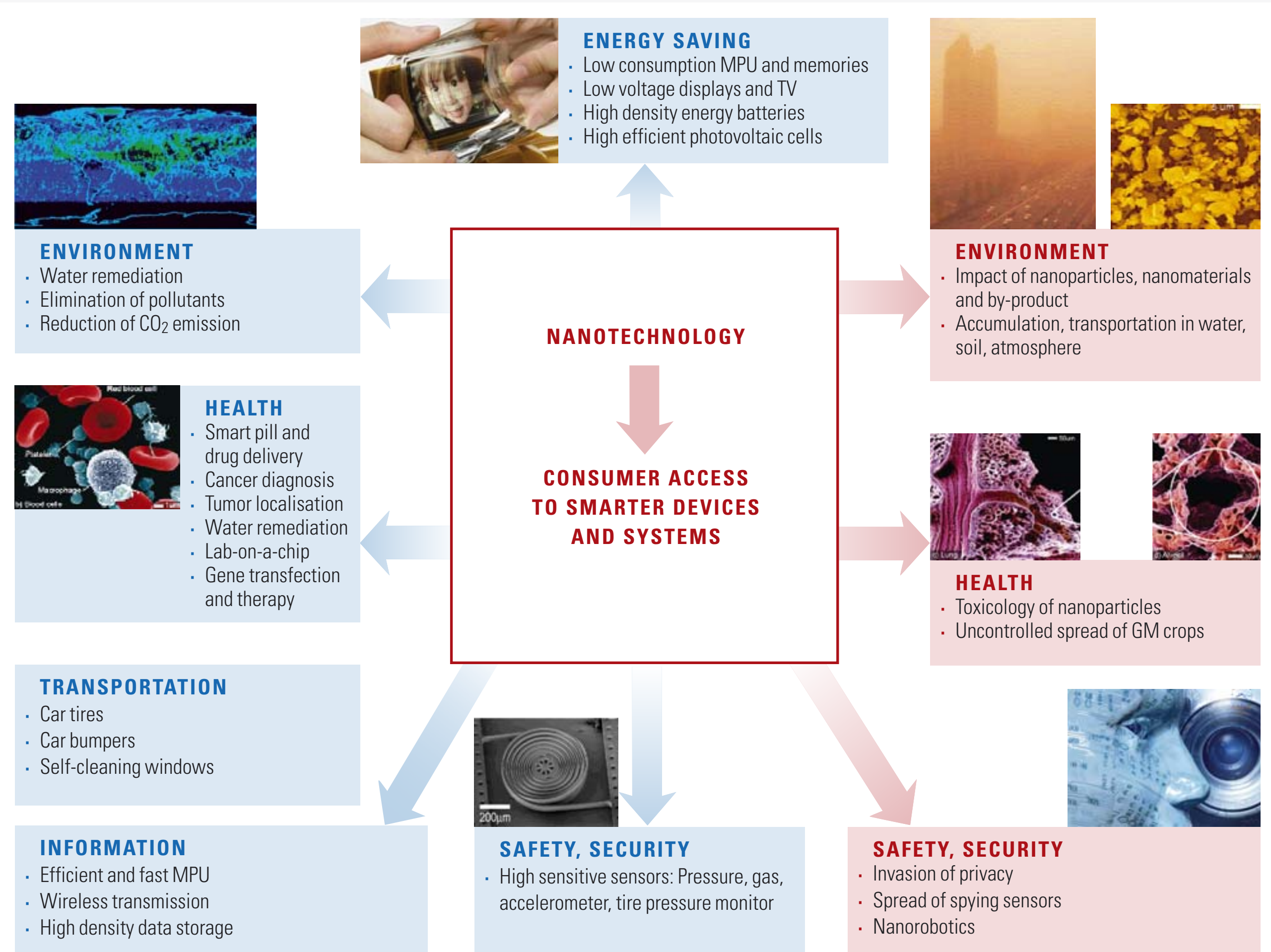


Fig. 11.10.1: Benefits and risks of nanotechnology; some examples.

ment in order to prevent any misapprehension of the nanotechnology industry:

- To educate the general public about science and nanotechnology. This education can be envisioned either at primary school or at college. Teaching children about nanotechnology is a great tool to indirectly inform the general public as well.
- To accurately and frequently inform the general public about the benefits, risks and probabilities associated with nanotechnology. Dissemination of information to the public must be transparent, reliable and performed by all participating actors: stakeholders, including public interest groups, scientific community, nanotechnology manufacturers and public authority (Fig. 11.10.2).

Finally, a global understanding of nanotechnology specific risks and benefits is fundamental if large and small industries are to operate on a level playing field, and developing economies are not to be denied essential information about safe nanotechnologies.

Role of large-scale synchrotron radiation and neutron facilities

Synchrotron radiation and neutron facilities must contribute to the assessment of the potential risks related to a specific nanomaterial and a nanodevice exploiting their analytical potential in almost any possible environmental condition.

The assessment and prevention of potential hazards associated with a specific nanomaterial or nano-enabled product will allow an accurate and reliable risk governance of the investigated nanosubstance, which must be carried out in close coordination with public authorities, industry and consumer for better efficiency.

Moreover, since national and European large-scale synchrotron radiation and neutron facilities are generally managed through international organisations, they can be considered as impartial and neutral organisms. Consequently, they are perfectly suited for educating the general public about science and nanotechnology, and for disseminating information about the research results concerning the assessment of risks and benefits of nanomaterials, devices and products (Fig. 11.10.2).

- **Conclusions**

The development of micro- and nanotechnologies will be highly beneficial for our society. The misapprehension of nanotechnology may create a general fear that nanomaterials and nano-enabled product are toxic. Nanoengineered material toxicity deserves some specific investigations. Due to their high spatial resolution and brightness, as well as their enhanced sensitivity, synchrotron radiation and neutron facilities will be increasingly useful not only in characterising advanced nanotechnology processes, but also in assessing, minimising and preventing the potential risks associated with any nanomaterial and nano-enabled product. Nevertheless, some noticeable enhancements are compulsory for enhancing the spatial resolution and sensitivity of current instruments in order to keep in pace with the very fast development of nanotechnologies and engineered nanomaterials.

Since national and European synchrotron radiation and neutron facilities are international, they are ideally suited for disseminating accurate and transparent information about the benefits and risks of nanomaterials and nanodevices from their initial manufacturing step and public use, to their final disposal.

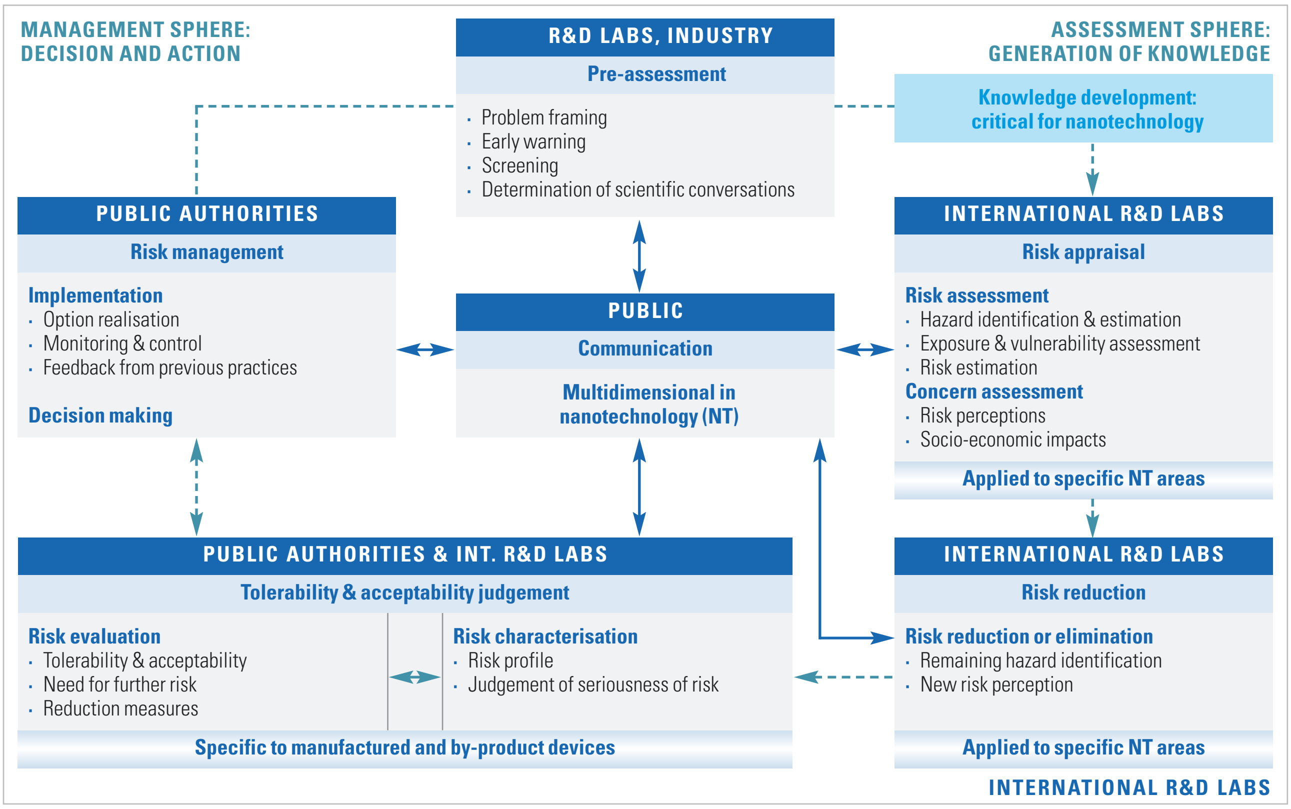


Fig. 11.10.2: Risk assessment and management framework for nanotechnology (NT).

11.11. GENNESYS SCIENCE AND TECHNOLOGY CENTRES

The creation of nanoscience/nanotechnology centres of excellence represents one of the efficient replies for organising the stakeholders, within a limited number of centres with a critical mass of interdisciplinary and intersectorial knowledge and research infrastructure to make a substantial impact in the field. The main objectives of such a centre are:

- To pull together the leading experts from all sectors (research labs, universities, research infrastructure, industry) and from all European member states to work in an optimised environment on an urgent area of nanoscience and -technology;
- To develop in this area a European excellence hub as well as a knowledge and service platform in research and education for academia and industry;
- To collaborate with the European research infrastructure in a strategic way;
- To collaborate with the European universities and the European Nanoscience College in the research-focused education of nanoscientists and nano-engineers;
- To stipulate – as a European hub – a strategy for global cooperation in research fields of global dimension (energy, environment, climate, diseases).

This mission of a centre should be underpinned by a new strategic access of the centre to the European accelerator-based x-ray and neutron facilities and by several transverse rooms which provide technology transfer schemes and professional help in IPR issues to stipulate efficient academia-industry cooperation as well as start-ups (see Fig. 11.11.1). Furthermore, the centre should be involved in a European education strategy in nanoscience.

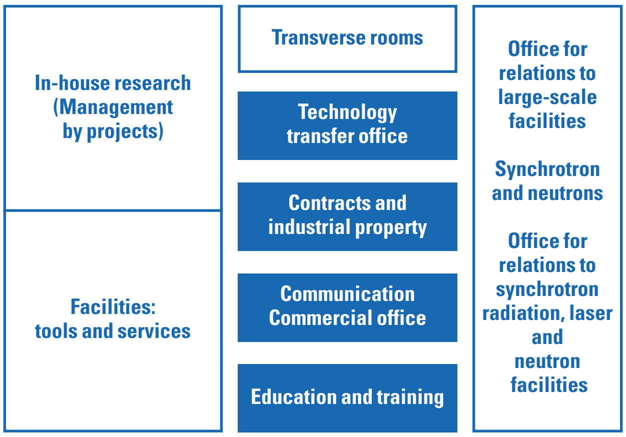


Fig. 11.11.1: Possible set-up for GENNESYS Science and Technology Centres.

Each centre should be given an appropriate legal status taking into account preferences by the hosting country. Each centre should be opened to external projects from academic institutions and industry.

The activities encompass:

- Design and operation of the analytical technology located at the large-scale facility;
- Coordination of the specific nanomaterials research programme;
- Assistance of external users before, during and after the experiments;
- Participation in the European nanoscience education programme;
- Development of a Hub function for international cooperation (USA, Asia);
- Information about the centre and the large facilities techniques;
- Transfer of knowledge to industry.

The GENNESYS document proposes Centres of Excellence in Softmatter materials, Food Science, Structural Nanomaterials, Nanomaterials for Energy, Nanomaterials for Cultural Heritage.

11.11.1. EUROPEAN CENTRE FOR STRUCTURAL NANOMATERIALS

This report has documented how a suite of neutron and synchrotron techniques can illuminate modelling and fabrication strategies leading to the identification of radically improved structural materials operating in new regimes of timescale and environment. Furthermore, they require the confluence of disciplines, fabrication and analytical techniques not found within a single laboratory. Europe has some of the best facilities in the world, it is essential that these are employed strategically.

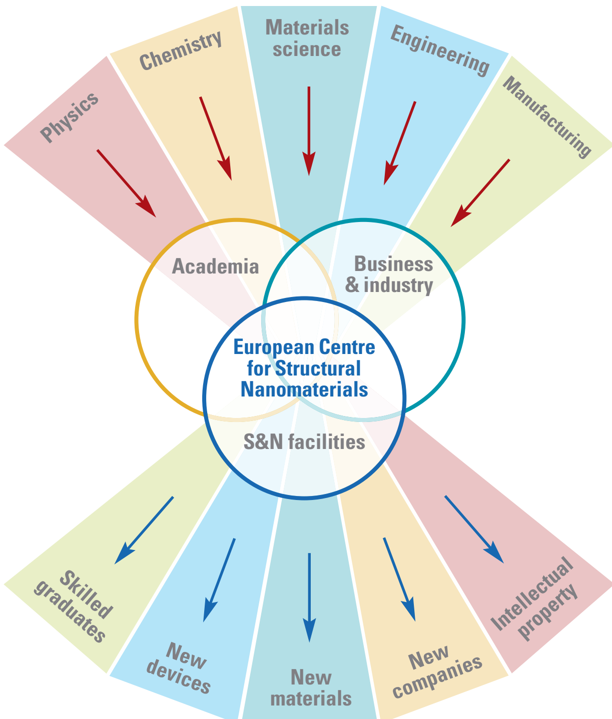


Fig. 11.11.2: Inventing and studying new materials at the nanoscale requires the exploitation of neutron and synchrotron techniques to better characterise their structure and monitor their performance in real-time under realistic condition. This will require a bold rethink about how academic and industrial R&D comes together with instrument scientists. A European Centre for Structural Nanomaterials could be an engine for invention.

The creation of a European Centre for Structural Nanomaterials would enable multi-disciplinary teams to develop roadmaps charting the route from basic physics through to fabrication of real prototype devices (see Fig. 11.11.2). It is necessary that it should bring together academics, industrial researchers with instrument scientists to plan and schedule experimental programmes. Furthermore, it is mandatory for the Centre to have a direct access to neutron and synchrotron radiation beam lines. Significant funds should be invested in rigs enabling the study of nanofabrication processes, nanostructures, as well as the structural and functional performance of materials and devices under realistic environmental and industrial conditions. A dynamic multi-disciplinary spectrum of permanent staffs should be complemented by academic visitors and industrial secondees. The site should host an incubator for fostering spin-out companies exploiting new technologies and devices developed by the Centre.

Currently, the capability to invent, manufacture and monitor new nanomaterials and devices are implemented as serial operations. To design really radical materials and devices one needs the design, fabrication, characterisation and performance evaluation capabilities to be brought together on one site in order to remove the barriers between these different activities and to increase the interactivity between the functions. Only in this way, step jumps will be realised ahead of the competition world-wide (see Fig. 11.11.3 and Fig. 11.11.4).

Such a Centre must be co-located within proximity to large-scale neutron and synchrotron facilities. The features of such a centre include:

- Nanofabrication facilities to manufacture and assemble nanostructures and prototype devices;
- Instrument scientists for the development of dedicated characterisation and in-situ monitoring tools;

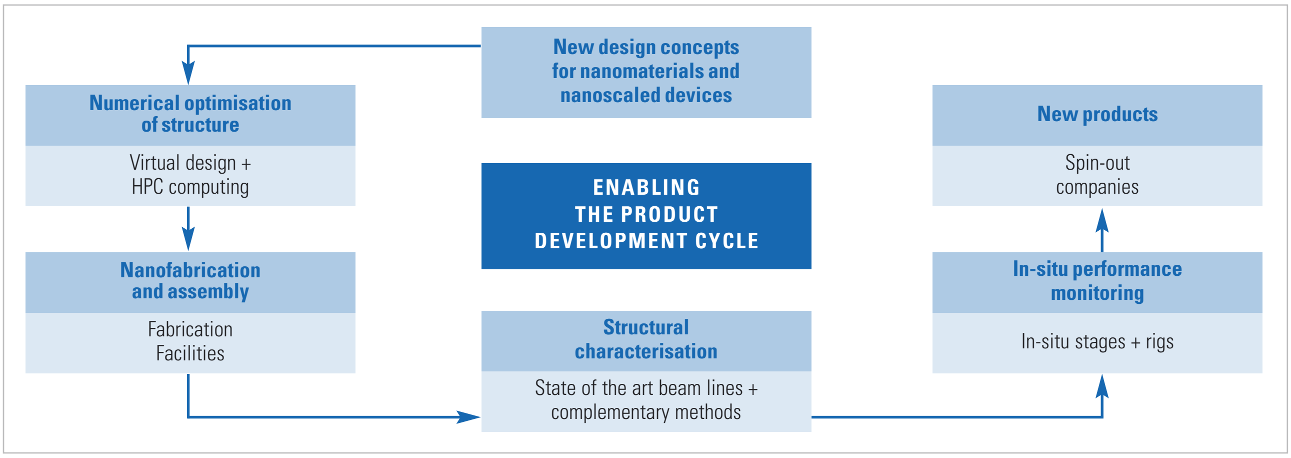
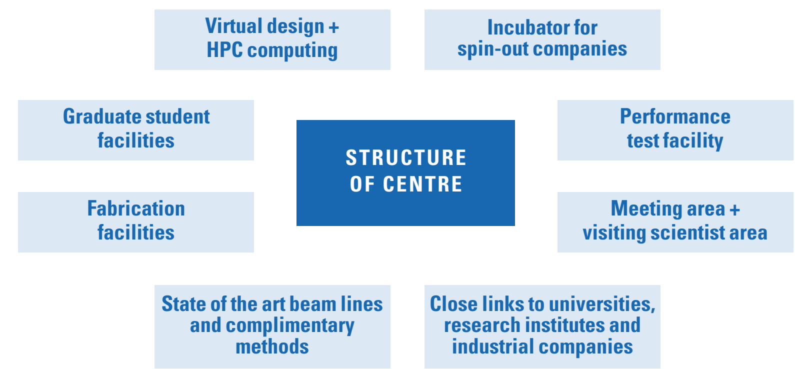


Fig. 11.11.3: Future research strategy for enabling the development of products based on nanostructural materials.

	Area (m^2)
Computational materials design suite	300
Nanofabrication space	300
Characterisation facility	400
Performance test facility	400
Data storage	25
Consumables storage	120
Cellular offices	180
Meeting area	130
Reception	125
Circulation space (corridors)	400
Breakout space	20
Meeting rooms	240
Local storage	150
Total area (m^2)	**2,790**
Total cost (€)	14,648



Facilities: To equip the Centre would cost around € 25M for nanofabrication, computing, test and evaluation facilities.

Operating Costs: Neglecting the amortisation of equipment and the purchase of new facilities, the Centre would cost around € 15M per year to run.

Fig. 11.11.4: Possible structure for a Centre for Structural Nanomaterials and an estimation of the incurred costs.

- Test labs for creep, fatigue, wear, strength, corrosion, high-T behaviour;
- Office and transport for visiting fellows and PhD students from collaborating universities and institutions;
- Training facilities for Master´s and PhD courses;
- Virtual design capability to optimise and develop designs;
- Partner companies interested in nanodevices and structures;
- Spin off companies to exploit new technologies.

11.11.2. EUROPEAN NANO/BIO-SOFT MATTER CENTRE

Soft-condensed matter has developed a strong interface with chemistry and biology and has become closer to nanoscience and materials science. Nowadays, highly dynamical (for example molecular motors), hierarchical systems and bio-inspired materials or systems are considered, with applications in several fields like cosmetics, food industry, pharma industry, biomedical applications, paints, lubricants to microelectronics, microfabrication, solar cells and bone substitutes. Generally, nano-/bio-soft-condensed matter concerns directly industrial sectors such as energy, medicine, cosmetics, food, and others manufacturers involved in specific equipments or instrumentation.

The challenges for the scientific researches for the next 15 years in Europe, described in the preceding chapters were also analysed in the conclusions of the White Book on "Polymer Nanoscience and Nanotechnology: A European perspective" produced by the NoE NANOFUN-POLY. The main goal is to be able to develop transdisciplinary research combining organic, macromolecular, as well as inorganic chemistries, modelling and simulation, biology and biotechnologies, materials engineering, and environmental sciences. Combination of efforts in integrated approaches from molecules or nano-objects to devices for strategic industrial applications is required to turn the conventional industry to a knowledge- and high value based one. The integration of soft matter, functional nanomaterials and nano-objects into devices will be deployed in close collaborations with other European centres dedicated to specific fields as for example the one involved in nanomaterials and nanotechnologies for Energy but requires building a specific European centre dedicated to nano/bio-soft matter activities.

This centre should be focused on the search of new concepts, new design of soft-matter nanostructures and bio-inspired nanomaterials. A collaborative academic/industry platform will offer both in-house specific and innovative tools (advanced synthesis, deuteration and processing, surface and interfacial engineering, electron microscopy, IR, AFM, confocal microscopy 3-D microscopy – tomography – reflectometry) and access to synchrotron and neutron facilities (see Fig. 11.11.5).

The ambition of this European centre is to provide all multi-disciplinary competencies and state-of-the-art tools to develop world class research in the nano-/bio- soft matter domain, which cannot be found elsewhere. As the development of complex hybrid materials requires non-conventional characterisation and monitoring concepts, the location of this centre in close neighbourhood to a synchrotron radiation, laser and neutron facility is an essential criterion. This academy/industry platform will offer all services necessary to design nanostructures and bio-inspired materials.

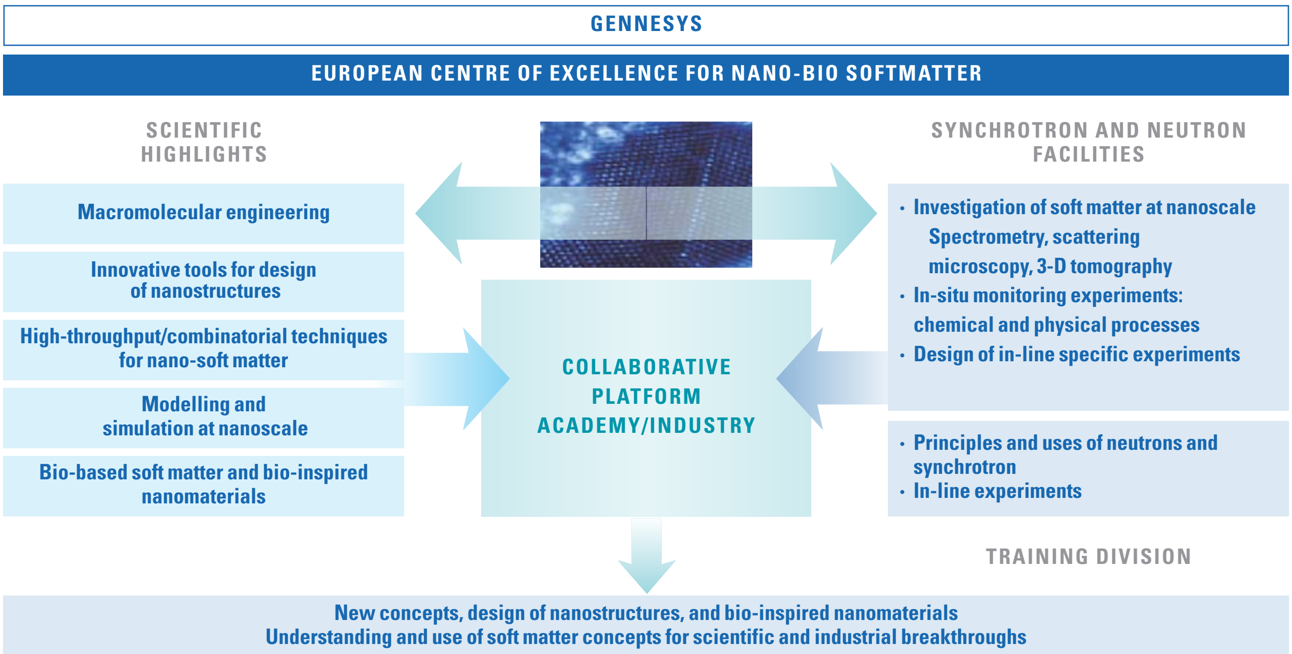


Fig. 11.11.5: Possible set-up for a European Centre of Excellence for Nano-Bio Soft Matter.

11.11.3. EUROPEAN NANOFOOD SCIENCE CENTRE

Food science and technology have started to profit from parallel developments made in SCM (Soft Condensed Matter), materials science and nanotechnology. Our understanding of complex food systems has made considerable progress in selected areas due to the application of analogies drawn from classical soft condensed matter sciences, combined with the use of novel techniques that allow non-invasive and time-resolved investigations of complex, soft and fragile food systems.

Future food research must take advantage of the enormous progress made in materials science, nanoscience and -technology, soft matter physics and chemistry, and of instrumentation at large-scale facilities. This can be achieved by a European research centre, which would have to be built based on the following key areas with the connections to different science fields (see Fig. 11.11.6):

- **Soft condensed matter science** (food colloids, food polymers and food surfactants):

This will not only allow to create important synergies among these areas, but result in new ways of creating food systems with tailored properties through the utilisation of novel concepts in areas such as aggregation, crystallisation and gelation that have been developed in soft condensed matter physics. The equilibrium and non-equilibrium properties of colloids, emulsions, foams and gels are areas where soft matter physicists and chemist intensively have been working on, and important progress can be made with the consideration to food structure and stability. Moreover, soft matter physicists have conventionally heavily used large-scale facilities and have pioneered the applications of neutron and x-ray scattering to their systems. They will thus be able to help develop new experiments and facilities that will be instrumental to extend the traditional food scientists tools and utilise state-of-the-art facilities in order to study food samples at all levels of structures from the nano- to the mesoscale.

- **Advanced non-destructive characterisation tools**

This multi-disciplinary centre should create a state-of-the-art infrastructure with the necessary nanotools (e.g. atomic force microscopy, electron microscopy, neutron, x-ray and light scattering techniques) which indispensably permit to analyse and understand the complicated molecular architecture, behaviour of proteins, polysaccharides, lipids, food colloids and their structuring principles in terms of complex food matrices.

- **Nanomaterials competence**

The multi-disciplinary design of the institute will also give countenance to an activity in nanomaterials that will play a major role in the form of nanocomposites in packaging and protective coatings (improvement of barrier properties). Furthermore, "intelligent materials" might be used for food monitoring (integrated quality indicators alerting a consumer about contamination and/or presence of pathogens, invisible nanotags for product traceability). A target is to develop cheaply and highly integrated diagnostic systems of higher sensitivity, specificity and reliability for chemical, biological and medical analysis should be established.

- **Functional food**

In the development of so-called functional food, the concepts from traditional food science, nutrition science and pharmaceutics meet. This is an area where nanotechnology (nanomedicine) and food sci-

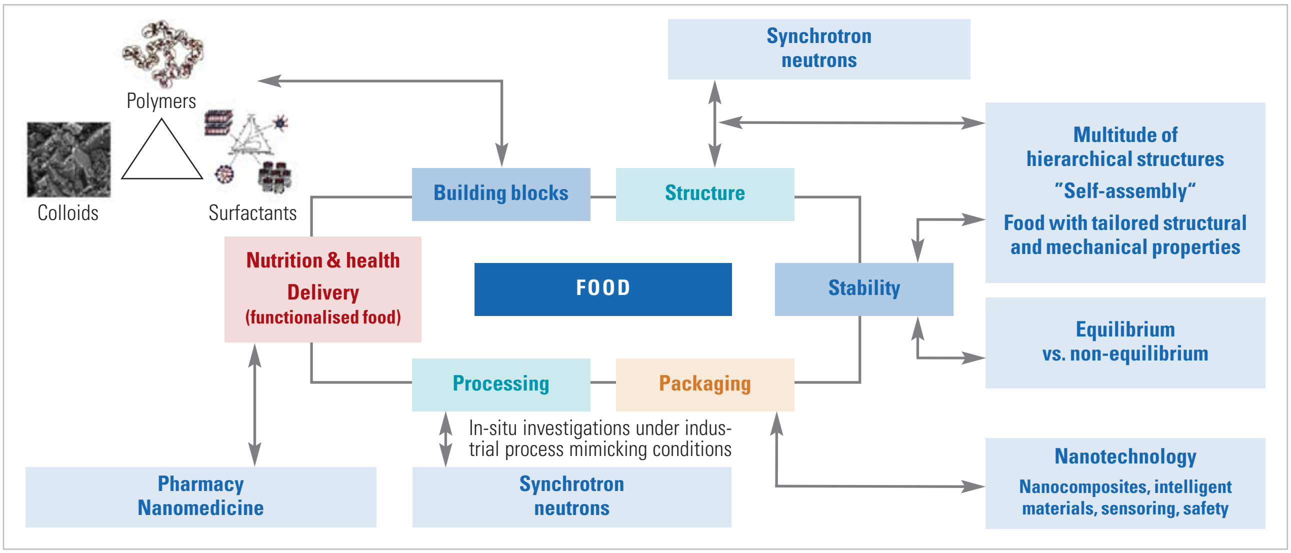


Fig. 11.11.6: Summary of key areas to be covered in a European Nano- and Food Science Centre. The colour code indicates the links to soft matter science (blue), areas where large-scale facilities will have a particularly important influence (green). Moreover, nanotechnology will make a direct and positive impact that will be met potentially with some reservation from consumers thanks to the discussions on the chances and risks of nanomaterials (orange), and areas connects to nanotechnology, pharmaceutical science and nanomedicine which could bring important progress. Nevertheless, the industry will be very reluctant to participate because of consumer concerns.

ence meet directly. Food industry is however very reluctant to enter this domain due to the consumers´ concerns. The centre could therefore play a key role in an area that could have enormous social, medical and economical impacts when looking for example at all the problems connected to nutritional deficiencies encountered particularly in developing countries.

The requested multi-disciplinary nature of the centre and the direct access to large-scale infrastructure allow designing experiments under processing conditions. The motivation to teach the future generation of food scientists has to be grown in a truly multi-disciplinary environment that clearly indicates the demand for a European dimension that such an institute should have. The centre would mainly profit from a close connection to a neutron and synchrotron facility, and should be directly involved in running dedicated beam lines for its own research staff and a corresponding user community that is expected to grow significantly.

The centre should offer world class working conditions in order to attract leading scientists. A working model for the centre's organisation could be based on research activities which will allow it to not only perform a rigorously fundamental research program, but also develop the socio-politically important role of a think tank and research centre for innovative SME's and national and international companies and public bodies and assure substantial funding of its running costs after an initial period when the infrastructure will be built up with European and national funds: i) fundamental science financed by European and national funding agencies and ii) long-term applied research financed by industry or jointly with European programmes. It will be crucial to secure an interdisciplinary composition (physics, chemistry, biology, materials science, food science, nutrition) of its staff, excellent basic equipment and open access for industrial partners. Another important aspect will be the creation of structures that bring an efficient technology transfer. The centre should generate an open laboratory structure with a visitor's programme where scientists can visit at various times to perform experiments at the centre. The open lab will be combined with an application laboratory for industry as well as the possibility of having mixed groups between industry and the centre. These different initiatives will help to create a vibrant scientific atmosphere and generate new collaborations between the institute and external groups.

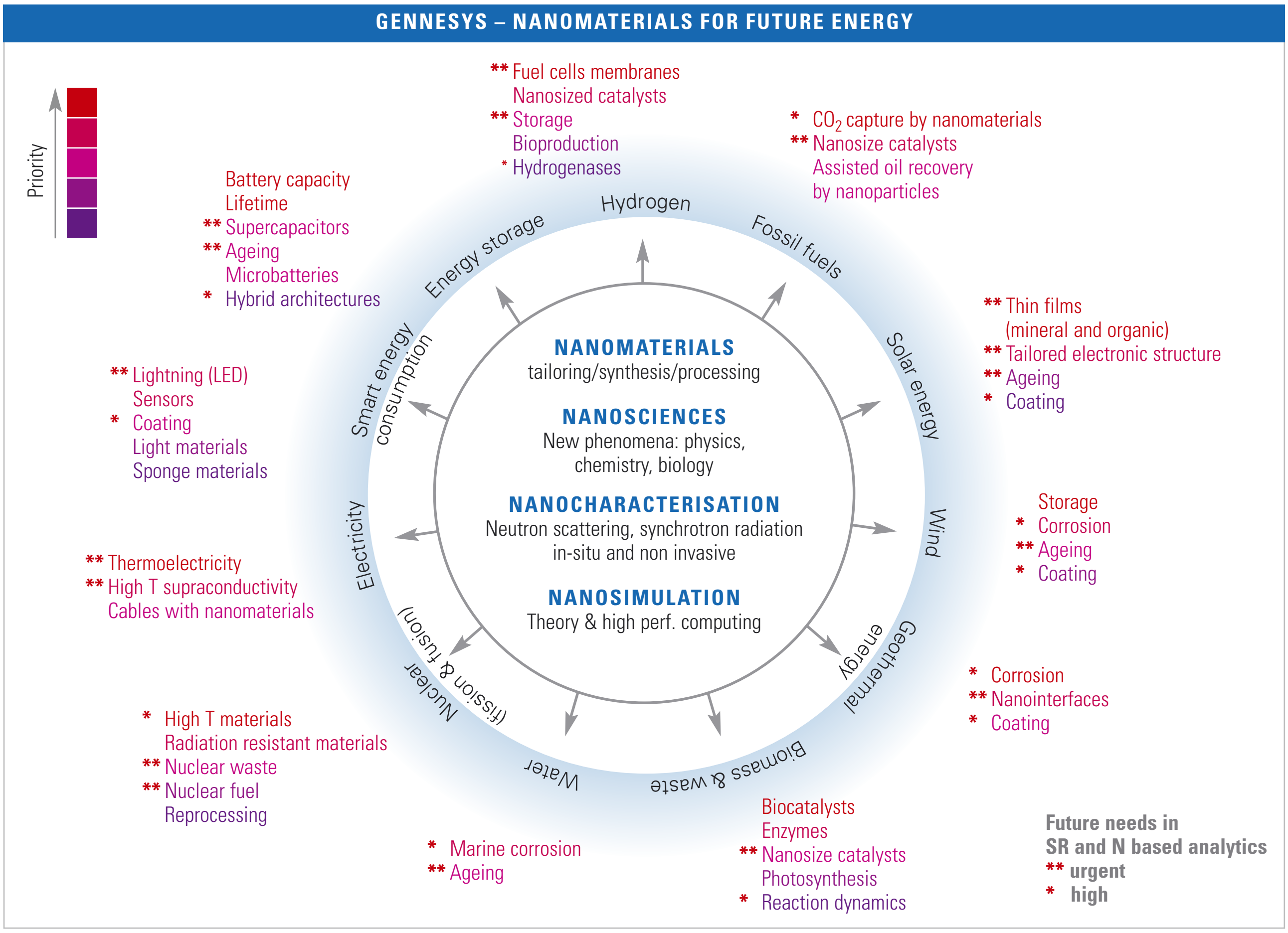


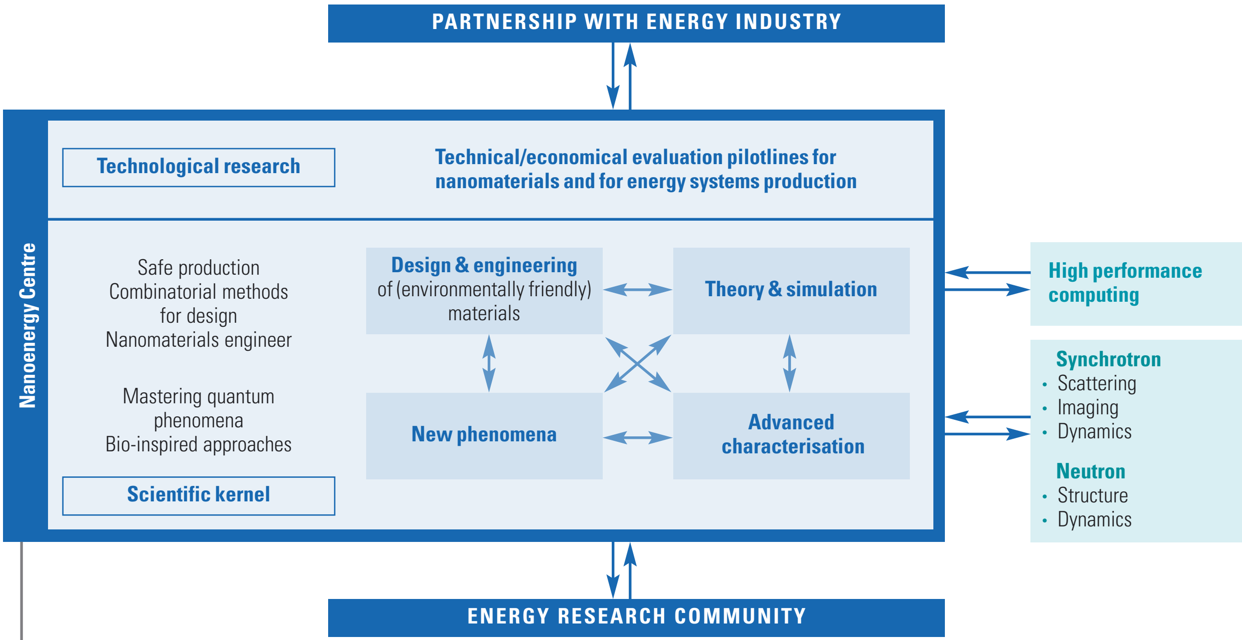
Fig. 11.11.7: Research infrastructure for energy materials.

11.11.4. EUROPEAN CENTRE FOR NANOMATERIALS FOR ENERGY

A robust European research programme in energy materials is clearly essential to ensure the technological breakthroughs that are required to meet the European emission reduction and supply targets (see Fig. 11.11.7 and Fig. 11.11.8). The programme must be broad enough to cover the diversity of materials which play an essential role here.

The research programme needs to address the different timescales involved in the different fields.
These timescales are:

- Short-term: present to 2020;
- Mid-term: 2020–2050;
- Long-term: 2050–2100.



Domains of research for Europe in the field of nanomaterials for energy

DOMAIN	THEORY & SIMULATION	TAILORING, SYNTHESIS & PROCESSING MATERIALS
Solar energy	Tailored electronic structure, excited states simulation	Thin film (organic and mineral)
Biofuels		C_5 sugarhydrolysis 2nd generation (demonstrator) Algaefuels
Nuclear energy	Multiscale modelling Propagation of nanodefects	Nanomaterials contribution to materials under extreme condition (radiation, temperature)
Energy efficiency	Modelling phenomena, Simulating complex systems	Nanostructured materials for thermoelectricy, lightning, high Tc superconductors
Storage	Modelling ageing	Nanomaterials for batteries electrodes and supercapacities
CO_2 capture and sequestration	Modelling transport phenomena	Nanomaterials carbonation of CO_2 Large-scale demonstrators
Hydrogen	Modelling transport phenomena and ageing Modelling bio-systems used for bio-production	Nanostructures and nanomaterials for fuel cell membranes and storage bioproduction

Fig. 11.11.8: Possible set-up for a European Centre for Nanomaterials for Energy and the involved domains of research for energy.

The short-term research should be aimed at the commercialisation and deployment of current technologies, directing such topics as durability and cost in fuel cells, high energy density batteries, supercapacitors, and the continued development of catalysts for hydrocarbon reforming and processing etc. The mid-term programme should include goals such as the development of hydrogen storage media for transport applications; innovated solar cells, improved superconductors, materials for next generation fission reactors. The long-term goals focus on such topics as materials for fusion reactors, high temperature electrolysis cells and materials aimed at the hydrogen economy.

There will be a growing demand for in-situ studies of the behaviour of new materials under operating conditions (i.e. aggressive environments; high temperature, high pressure, corrosive etc.). A summary of this strategy is shown in Fig. 11.11.9.

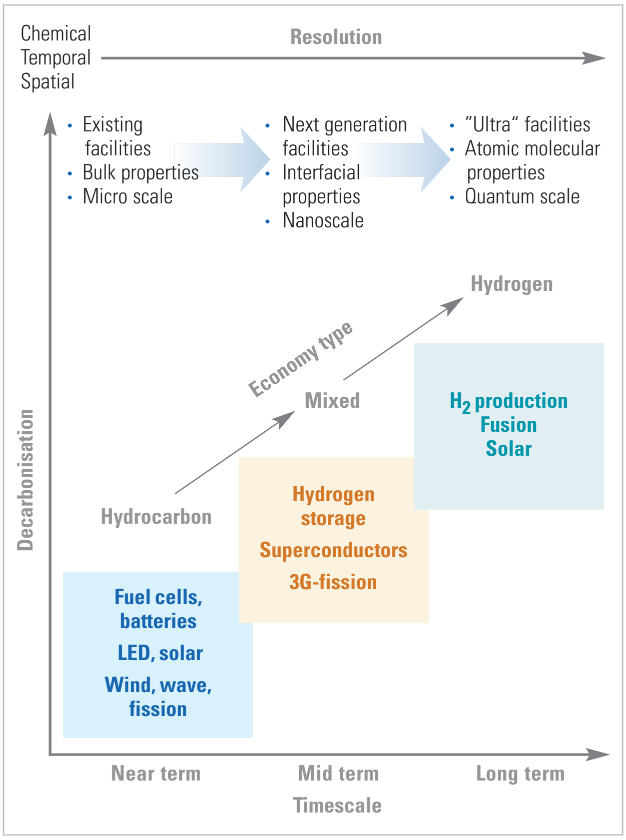


Fig. 11.11.9: Summary of the research strategy for energy technology.

Complementary to this development in characterisation techniques, there will be the demand for high performance computing. There will be an increasing need for high resolution visualisation of atomic and sub-atomic scale processes. It is almost trivial to emphasise that modern experimental techniques could not exist without the concomitant increase in computational power.

If we have ever achieved the aggressive targets set by the European Union in preserving the necessary economic base whilst protecting the earth's climate, it is important that scientists and technologists in Europe have uncluttered access to cutting edge characterisation facilities that will enable them to deliver the requisite set of novel and exciting new materials.

11.11.5. EUROPEAN CENTRE FOR NANOMATERIALS IN CULTURAL HERITAGE

A European Centre for Nanomaterials in cultural heritage represents a direct response to the scattered scientific communities (archaeometry, paleontology, past environmenl sciences, conservation sciences) by bringing a bridge between disciplines, through a common interest to investigate materials on the micro- and nanoscale (see Fig. 11.11.10). The diversity of the materials (or objects) involved is very broad and includes biomaterials (bone, teeth, and fibres), sediment, ice cores, speleothems, painting materials, metals, stone and other building materials, wood, etc. These materials, most often made from natural ingredients and sometimes heavily altered due to long-term ageing, are highly heterogeneous. Each of these disciplines will benefit of the most advanced pluri-disciplinary research in micro- and nanoanalysis with top level competencies, which are out of reach by themselves alone. The potential of organisation, investments and competences, which is necessary prior to and after any use of large-scale facilities will offer a new dimension of research to a large number of scattered teams, thus strengthening European leadership in these domains. Furthermore, the art market, museums, or foundations, bodies involved in cultural heritage in general, could directly address themselves to the Centre and benefit from the competencies and expertise of the Centre. No such centre exists today in the world and this would be a unique institute of its kind, capable to develop and even explore the interface between academic research and societal needs in the cultural and art domain, such as museums or other bodies connected to the art market or to the cultural heritage tourism.

Over the past years, tremendous developments have taken place using micro-imaging techniques at large-scale facilities for the analysis of materials of cultural heritage interest. This research has focused on topics as diverse as the study of paint layer stratigraphies to retrieve technical art history information, the study of metal objects for conservation and archaeological provenance purposes, the 3-D imaging of paleontological specimens to deduce phylogenetic information, the study of sub-annual climate local variations by looking at speleothems. All these approaches benefited primarily from the new imaging capabilities (2-D, 3-D, 4-D) developed at the macro- and microscale. Europe today plays the leading role of the research at the interface between synchrotron/laser/neutron techniques and ancient materials.

Based on today's cutting-edge research and expected breakthrough for the decades to come (see Chapter 5.11.), these areas of research would strongly benefit from innovative coupling between micro- and

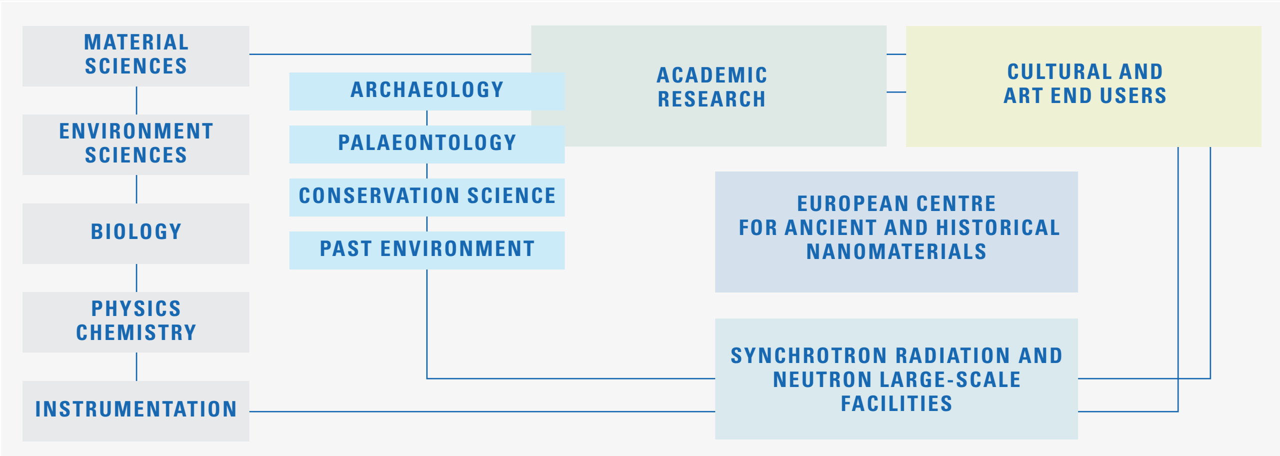


Fig. 11.11.10: Possible set-up for a European Centre for Nanomaterials in Cultural Heritage.

nanoscale characterisations. Nanocharacterisations currently involve pilot studies that could rapidly evolve at a much major scale provided adequate instrumentation and support are put in place. For this purpose, synchrotron radiation and neutron centres will bring the unique opportunity to combine micro- and nanocharacterisation and could consequently facilitate characterisation and integration of the information at the successive length scales.

This Centre will grant access and expertise for state-of-the-art imaging and microscopy techniques to the ancient materials research community, based on two major modalities as follows:

- Develop innovative collaborative research activities on ancient materials and their environment, focusing on projects with an interdisciplinary character which cannot easily develop elsewhere and also on projects involving academic researchers and end users in culture and art;
- Offer various analytical instruments to prepare further studies with synchrotron and neutron facilities;
- Develop new instruments and methods such as imaging, microscopy techniques and data processing methods, including modelling at the nanoscale on analytical methods, behaviour laws, mechanical models, etc.
- Offer specific facilities for the storage and transportation of ancient specimens, objects, artworks and samples according to museum standards. Compliance with museum standards should be ensured for areas where artwork will be stored, even temporarily, or examined;
- Contribute to sharing the expertise among users, collect information, organise training events, disseminate to the end-users and to the public.

Regarding access, several options are considered in parallel:

- Access to in-house instrumentation developed at the Centre;
- Dedicated beam lines at LSF's nearby the Centre;
- Distributed privileged access to specific and multipurpose beam lines at LSF's (including distant facilities).

In addition, specific additional facilities will be available:

- Preparation rooms, including a specific sector for biologically sensitive samples;
- Laboratory spaces for laboratory characterisation and sample preparation;
- Training rooms and spaces for organising scientific and dissemination events;
- Area for the storage and transportation of ancient specimens, objects, artworks and samples according to museum standards.

11.12. GENNESYS ORGANISATION

The European action plan which has to be implemented to respond to the challenging GENNESYS conclusions and recommendations requires that an efficient GENNESYS organisation is created. In Fig. 11.12.1 a scheme is developed how the GENNESYS initiative should be integrated into the European research landscape. It is apparent that the realisation of the ambitious GENNESYS initiative requires strong efforts from different bodies and European institutions:

European Commission

- Promotion/catalysing the governments of the European member states;
- Implementation of appropriate actions;
- Implementation, coordination and operation of Centres of Excellence.

Governments of the European member states

- Allocation of funds for fundamental research and development in the frame of GENNESYS.

European Research Centres (ESF)

- Nanoscience programmes;
- Promotion of young scientists;
- Create public awareness/acceptance of fundamental research in nanoscience;
- Continuous update of the GENNESYS roadmaps;
- Education of future scientists and engineers for nanoscience and nanotechnology.

European University Association (EUA, EIT)

- Adjustment of the educational concepts to the future needs of industry and society;
- Exploration of interdisciplinary and cross – sectorial learning/training schemes;
- Embarkment into pan-European networks/EIT;
- Partnering with GENNESYS/EIT.

European Research Infrastructures

- Opening of the analytical infrastructure to strategic research in nanomaterials developments;
- Development of dedicated instruments and access concepts;
- Development of user support facilities dedicated to nanomaterials synthesis, manipulation and complementary characterisation;
- Hosting of science and technology centres.

Industry (EIRMA, EACRO, COST)

- Responsible partnering with academic research institutes/universities to promote innovation in nanotechnology;
- Realise an open innovation scenario;
- Sustainable support of fundamental research and education.

It is proposed that the European Commission Research (ERAB and ERC) and ESF install expert groups/task forces and create a GENNESYS secretariat in Brussels/Strasbourg with the final goals:

- To develop a long-term European (ERA) nanomaterials strategy plan;
- To coordinate the European nanomaterials activities and research infrastructure of the different European countries within the GENNESYS frame;
- To optimise the competences/excellencies by bridging nanomaterials R&D&T in Europe together with the large-scale facilities.

It strongly suggested to install a GENNESYS Council which coordinates all aspects of GENNESYS. It should include leading representatives from all sectors involved in European research and education. The mandate of this council should be the implementation of the GENNESYS vision and the overall guidance of the pan-European integrated nanoscience programme.

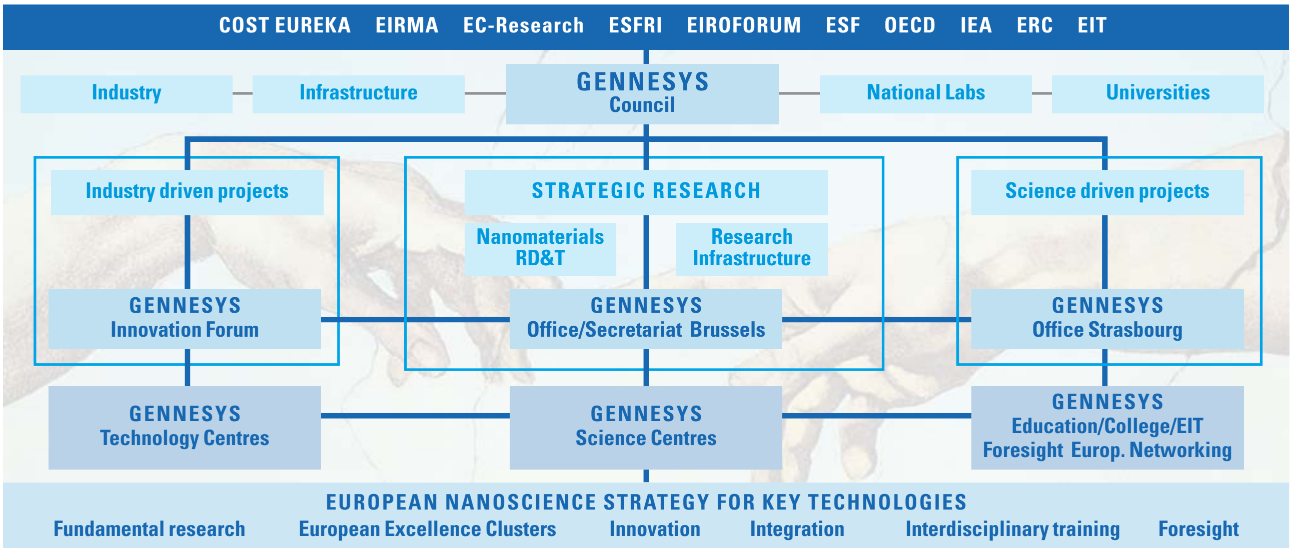


Fig. 11.12.1: GENNESYS organisation.

11.13. OVERALL CONCLUSIONS

Nanomaterials science and technology will provide breakthroughs for many technologies in the future, and solutions for urgent problems in our society. In order to leverage the fragmented knowledge in Europe for a strategic pan-European nanomaterials programme, a joint effort of all sectors of research and innovation is necessary, including the existing highly developed European research infrastructure.

A close collaboration between scientists, industrialists and the government is needed to safeguard this new nanomaterials research field. To stay competitive in a global market, to secure energy supply, and to meet the environmental challenges of our industrial society are the main socio-economic driving forces for the future development of European economy, and the potential impact and benefits of nanomaterials simply cannot be ignored.

GENNESYS is a foresight and strategy document compiled by using expert input from the education, science, technology, policy-making and governmental authorities. It has demonstrated that a stepwise improvement in Europe is needed in order to take a leading position in the world of nanomaterials science, technology and industrial exploitation. A strategy must be developed and delivered to ensure future impact on economy and society, and success in this grand challenging new world (see Fig. 11.13.1).

The conclusions of GENNESYS can be summarised as follows:

- The study gives an overall picture of the future research needs in the large spectrum of nanomaterials and highlights the important roles of advanced analytical equipment in reaching breakthroughs, especially the synchrotron radiation and neutron facilities. The study is a reference work for scientists, research managers, industrialists and policymakers to design new programmes and guide future research in nanomaterials.

- GENNESYS indicates the potentials for industrial innovations of nanomaterials; it gives directions for new targeted processing techniques. Synchrotron radiation and neutrons are ideal tools to measure progress in-situ.

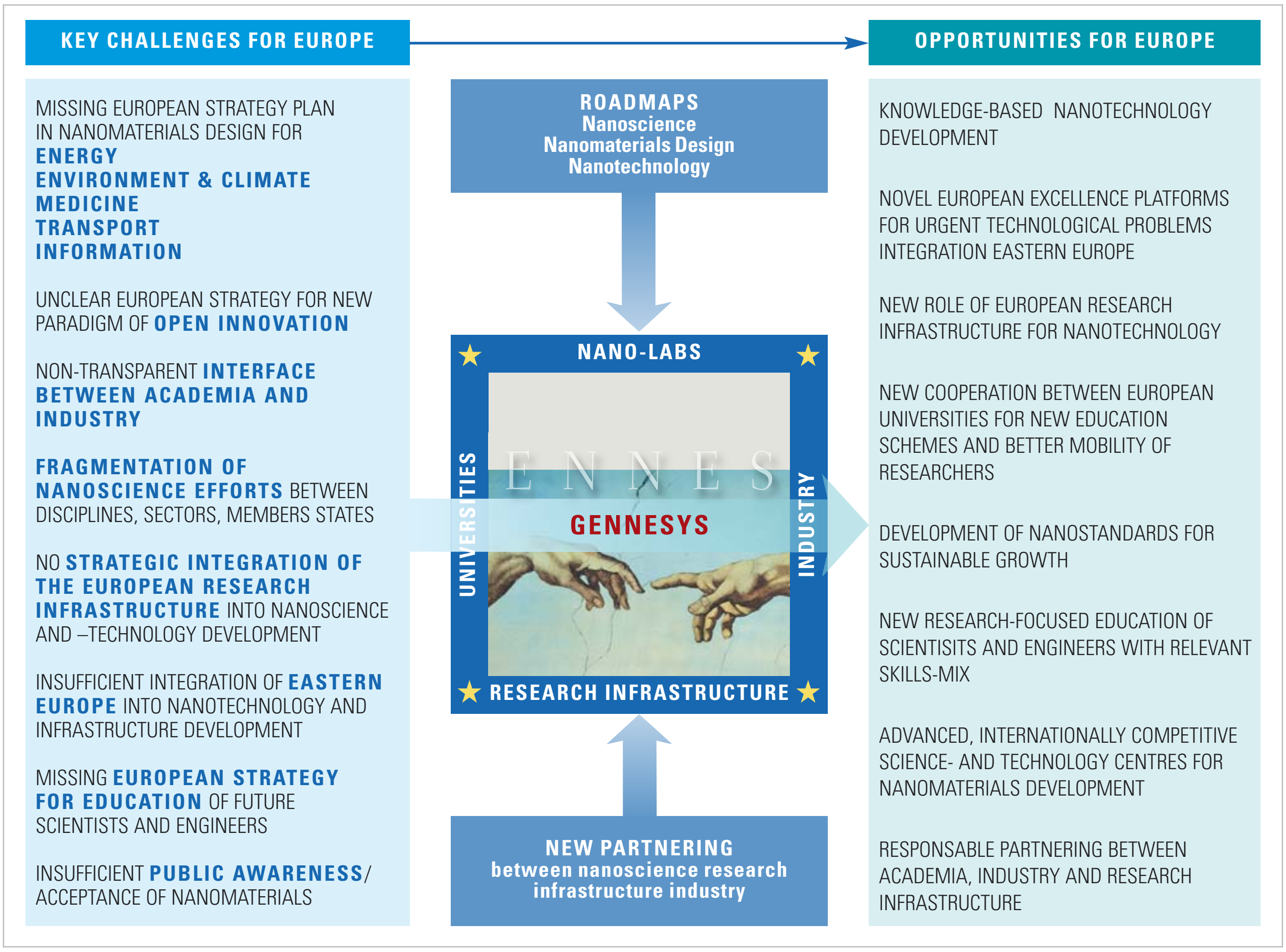


Fig. 11.13.1: Impact of GENNESYS.

- Nanomaterials research is thinly spread over many European countries and institutes. GENNESYS provides a mechanism to bring the efforts together in setting up GENNESYS Science and Technology centres throughout European at large-scale facilities. This is a necessity to keep Europe a forerunner in this field.

- The European GENNESYS Centres of Excellence bring the European talent together: scientifically, industrially, socially and economically (see Fig. 11.13.2). They are multi-disciplinary centres where nanoscientists from all European countries are welcome. They offer opportunities to research institutes and universities of central- and Eastern Europe to participate actively. The centres should have the theme of "Science" or "Technology" orientation. They could be compared to the CERN organisation in high energy physics in Geneva.

- GENNESYS highlights the importance of creating a European/international institution for nanomaterials where talented students could prepare for a brilliant career. This institution, with satellites around various large-scale facilities, recognised universities and industries, will become competitive with the best US and Japanese school in Nanomaterials. The institute should also deliver qualifications that are recognised throughout Europe.

- The GENNESYS study is analyses a wide spectrum of nanotechnologies. It hints towards solutions in the complex energy question, particularly related to new energy sources or to the improvement of existing sources. It also studied completely new topics such as nanomaterials for security and safety, nanopharmaceuticals and nanofoods, the role of "nano's" in global climate change, etc.

- The study pinpoints the advantages of nanomaterials but analysed in depth the research needs to combat the toxicology and nanoprotection problems and tries to delaminate the borders/boundaries between danger and no risks. Synchrotron radiation and neutrons are of great importance in studying the mechanisms of dangerous nanospecies in the body.
- In order to cope with the challenges and needs of nanoscience and technology, considerable improvements are needed also with

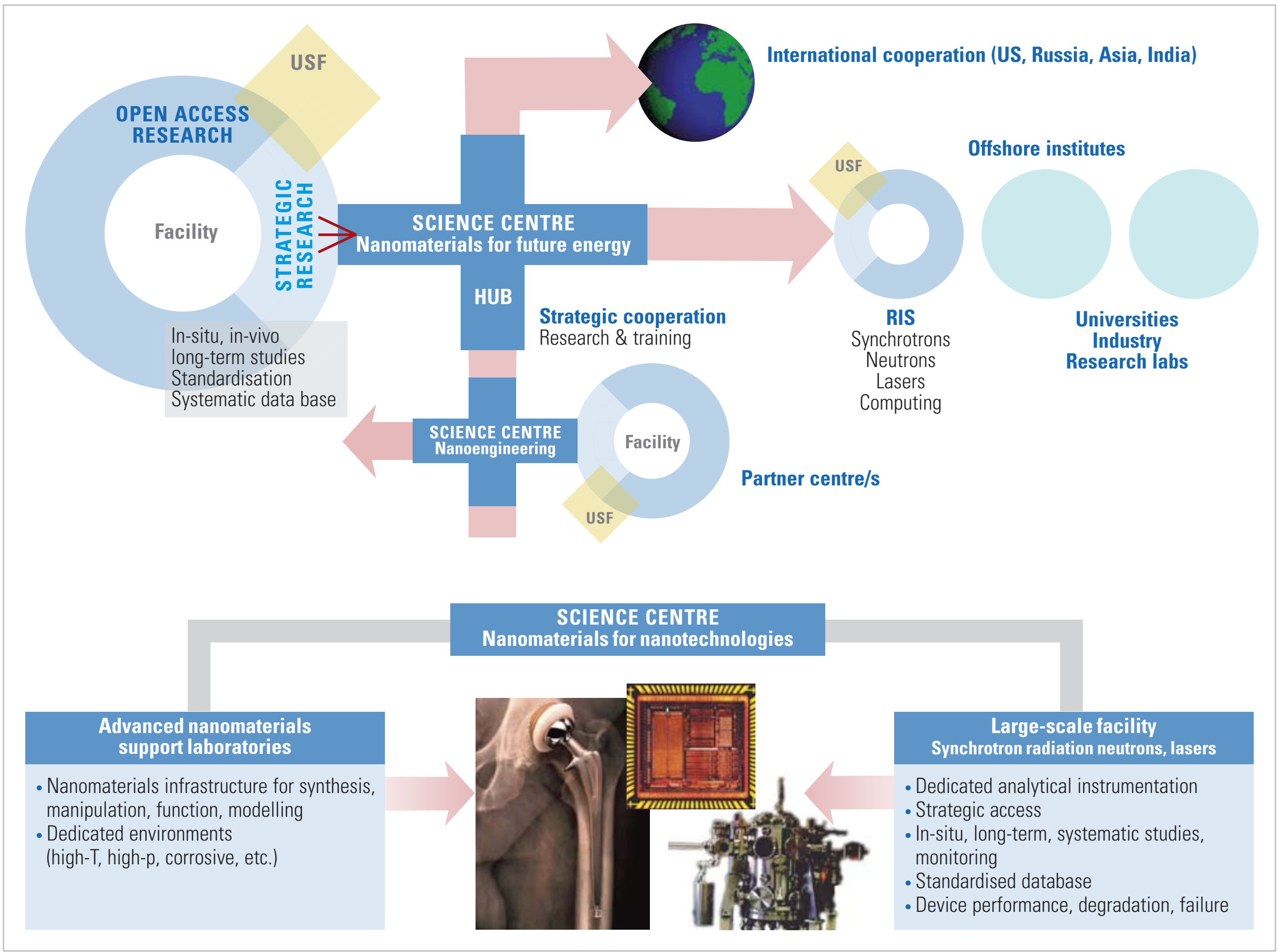


Fig. 11.13.2: Centres of Excellence and the strategic role of research infrastructure.

large-scale facilities such as synchrotrons and neutron sources. This has technical aspects as well as organisation aspects (availability, ease of access) and educational ones: e.g. extreme focusing, nanobeam stations, small neutron beams, transferring scientific results from laboratory conditions to realistic industrial ones.

To achieve efficient work and collaborations between large-scale analytical facilities and nanoscience and technology, the creation of GENNESYS type analytical centres is essential.

Europe will need to invest in the next generation of synchrotron radiation, laser and neutron facilities, offering higher fluxes and more brilliant probes, and providing significant and necessary advances with regard to resolution, sensitivity, and data acquisition. A continuous investment is needed in the upgrading of Europe's synchrotron x-ray sources, with improvements in equipment and instrumentation, new ancillary equipment to support new experimental methodologies, and a rolling programme of upgrades to ensure that Europe's synchrotron sources remain at the forefront of research in nanomaterials science and technology.

- It is suggested that the European Commission, in collaboration with the European Science Foundation and other European authorities and national and funding agencies, should establish a European body with the mandate to coordinate all nanomaterials activities and large-scale facilities in Europe.

- GENNESYS recommends creating a European College for Nanomaterials Science, Science Centres and Technology Centres of Excellence for research, development and exploitation of nanomaterials in closest interaction with the European research infrastructure. The European Synchrotron radiation, laser and neutron facilities have the most advanced analytical equipment and a solid and proven infrastructure of scientists and equipment.

- Governments should promote the creation of new European Centres of Excellence and an International Institute for Nanomaterials Education to be coordinated by the European Commission and/or relevant agencies.

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GENNESYS

GRAND
EUROPEAN INITIATIVE ON
NANOSCIENCE AND
NANOTECHNOLOGY

USING

NEUTRON- AND
SYNCHROTRON RADIATION
SOURCES

13. APPENDIX I: GENNESYS MEETINGS, CONFERENCES AND PRESENTATIONS

17TH DECEMBER 2002, GRENOBLE

Ad-hoc meeting of representatives from European nanoscience laboratories and synchrotron radiation and neutron facilities

AGENDA

1. Discussion on the development of nanoscience and -technology in Europe and the future role of synchrotron radiation and neutron facilities

2. Defining the objectives of the new GENNESYS initiative , namely:
   - 2.1. To assess the "state of the art" of nanomaterials science and technology
   - 2.2. To highlight future challenges and research needs, and order them in terms of priority and set out a suitable time frame for achieving them
   - 2.3. To pinpoint the areas of research into nanoscience and technology that will most benefit from joint research strategies with synchrotron radiation and neutron sources,
   - 2.4. To review and forecast the effects that increased use of large scale facilities by nanomaterials scientists will have on the facilities
   - 2.5. To formulate a European research strategy for "Synchrotron Radiation and Neutrons for Nanomaterials Science and Technology"

3. Further actions and Closing Technology

4. Preparation of a GENNESYS Document
   - 4.1. Operational structure of this initiative
   - 4.2. Installation of task forces
   - 4.3. Definition of the work of the task forces (roadmaps)

5. Discussion of further actions
   - 5.1. Short-term actions
   - 5.2. Mid-term actions
   - 5.3. Preparation of Kick-off workshop
   - 5.4. Presentation of document

6. Date of next meeting

7. AOB

26TH – 27TH FEBRUARY 2003, GRENOBLE

1st GENNESYS Meeting "Launching the Project"

GENNESYS

Grand European Initiative on Nanoscience and Nanotechnology using Neutron and Synchrotron Radiation Sources

AGENDA

1. Brief review of the initiative

2. Scientific Actions Taken (presentation of the current scheme and the priority areas)
   - 2.1. Pilotproject: Nanoscience and -technology
   - 2.2. Definition of "High Priority Research Areas (HPRA)"
   - 2.3. Identification of Nano research fields
   - 2.4. Identification of HPRA
   - 2.5. Preselection
   - 2.6. Integration of Key Labs and Authorities in EU
   - 2.7. Future Role of RIS

3. Actions to be undertaken

4TH – 5TH JUNE 2003, GRENOBLE

2nd GENNESYS Meeting "Getting Taskforces Started"

AGENDA

1. Welcome (Dosch)

2. Reports from the Task Forces
   - 2.1. Neutrons (Vettier)
   - 2.2. Synchrotron Radiation (Sette)
   - 2.3. Surfaces and Interfaces (Feidenhans'l)
   - 2.4. Nanosynthesis (Rossi)
   - 2.5. High Surface-Area Materials/ Catalysis (Magnus)
   - 2.6. Structural Materials (Steuwer)
   - 2.7. Functional Materials (Temst)
   - 2.8. Bioaspects and Biotechnology (Grunze)
   - 2.9. Information Technology (Davies/Whitehouse)

3. GENNESYS Discussion Session
   - 3.1. General Comments and Questions regarding generating Roadmaps
   - 3.2. Next Actions List
   - 3.3. Calendar: Meetings of GENNESYS and public GENNESYS presentations
     - 3.3.1. 25–26 September 2003, Grenoble: next GENNESYS Meeting
     - 3.3.2. 10–12 December 2003, Trieste: "Euro Nano Forum"
     - 3.3.3. 15–16 January 2004, Grenoble: Public kick-off meeting"
     - 3.3.4. 27–28 June 2004, Cork: "Materials Science and Technology Forum"

4. Summary

5. End of Meeting

25TH – 26TH SEPTEMBER 2003, GRENOBLE

3rd GENNESYS Meeting "First Results from Task Forces"

AGENDA

1. Welcome: DOSCH (DE)
   1.1. Introduction of new members
   1.2. Short introduction into the GENNESYS project
   1.3. Organisation of the meeting

2. Progress Report – Task Forces
   2.1. Materials Roadmaps
      2.1.1. Structural Materials: Kaysser (DE), Withers/Steuwer (UK), Mathiesen, (N)
      2.1.2. Polymers : Reynards (B)
      2.1.3. Functional Materials: Bruynseraede (B)
   2.2. Phenomena Roadmaps
      2.2.1. HSA/Catalytic Materials: Steinsmo (N), Jacobs (B); Hahn/ Weismüller/Pettenkofer (DE)
      2.2.2. Synthesis: Rossi/Cingolani (I)
      2.2.3. Thin Films and Coatings: David/Langridge (UK)
      2.2.4. Surfaces and Interfaces:Feidenhans'l (DK), Chesters (UK)
   2.3. Technology Roadmaps:
      2.3.1. Materials for the Information Technology: Müller (CH)
      2.3.2. Materials for Bio Technology: Grunze (DE)
      2.3.3. Materials for Food: Schenk (NL)
      2.3.4. Materials for Bio-Medicine: Di Fabrizio (I)
      2.3.5. Materials for Aeronautics – Transport and Mechanical Engineering: Kaysser (D), Withers/Steuwer (UK)
      2.3.6. Materials for Advanced Energy Technology: Stöver (DE)
      2.3.7. Pre-Normative Research: Bathias (FR), Adams (B)
   2.4. Facility Roadmaps
      2.4.1. Synchrotron Radiation Roadmap: Sette (FR)
      2.4.2. Neutron Roadmap: Vettier/Schober (FR)

3. GENNESYS and European Industry: Reynards (B), Jacobs (B)

4. Advanced Analytical Techniques: Role of Synchrotron radiation and Neutrons: Adams/Reynards (B)

5. GENNESYS Charter: Schober (FR)

6. GENNESYS Promotion
   6.1. Booklet
   6.2. Webside: Steuwer (UK)

7. GENNESYS Operation: Dosch (DE)

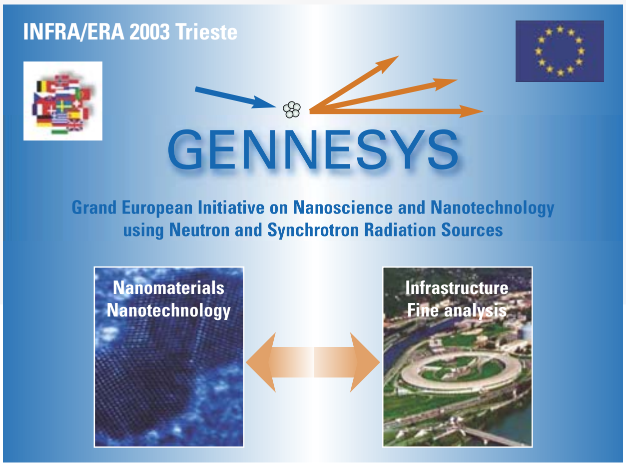
8. Internationalisation of GENNESYS

9. Planning of INFRA/ERA 2003 Trieste, Nov. 21, 2003: Dosch (DE)

10. Further Planning and Closing Remarks: Dosch (DE)

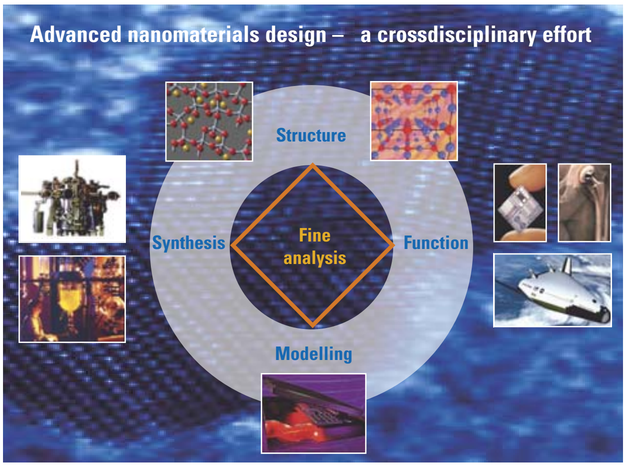
21ST NOVEMBER 2003, TRIESTE

GENNESYS Presentation at the E.C. INFRA-ERA Conference "Advanced analysis in nanospace: from fundamental research to new technologies" (Dosch)



3RD MARCH 2004, DIDCOT (RUTHERFORD LAB)

GENNESYS Presentation at E.C. Press Conference of Dr. J. Potoçnik Advanced analysis in nanospace: from fundamental research to new technologies (Dosch)



23RD – 24TH MAY 2004, STRASBOURG

5th GENNESYS Meeting “Progress of GENNESYS”

AGENDA

1. Reports from Task Force Leaders (Chesters, Feidenhans´l, Kaysser, Schober, Steinsmo, Tindemans)
2. Officialisation of GENNESYS (Dosch)
3. Preparation of the GENNESYS Kickoff Conference in Stuttgart
   3.1. Organisation (Bruynseraede, Dosch, Schober)
   3.2. Local Committee (MPI-MF, Stuttgart)
   3.3. Venue (Hotel Europe, Congress Centre Stuttgart)
4. Summary (Dosch)

24TH MAY 2004, STRASBOURG

Plenary GENNESYS Lecture at ESF Conference

Advanced analysis in nanospace: from fundamental research to new technologies (Dosch)

11 – 12TH NOVEMBER 2004, STUTTGART

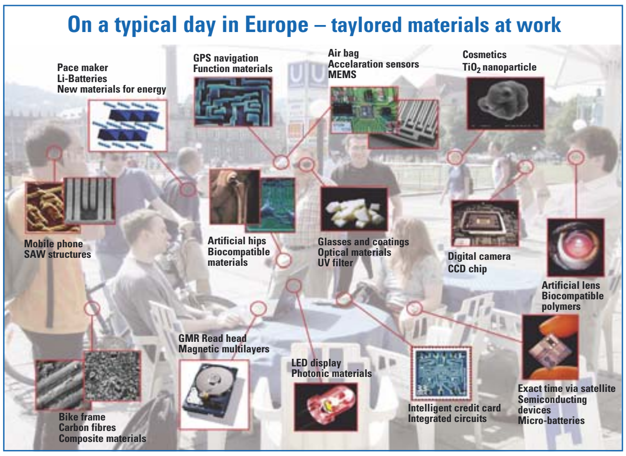
6th GENNESYS Meeting “Public GENNESYS Congress”

Sponsored by: FZJ, DESY, FZK, HMI, MPG

150 participants

AGENDA

1. Opening (Dosch)
2. Welcome adresses by:
   Dr. H. Knorr (Ministry Baden-Württemberg)
   Dr. A. Mitsos (DG Research, European Commission)
   Prof. K. Mehlhorn (Vice president MPG)
   Prof. E. Rytter (Special Advisor, Statoil – R & D)
   Dr. A. Monk (Nanomaterials, European Commission)
3. European Research Infrastructure
   3.1. H. Pero, (European Commission)
   3.2. H. Chang (Chairman ESFRI)
   3.3. M. Bertolo (Chairman Synchrotron Round Table)
   3.4. R. McGreevy (Chairman Neutron Round Table)
4. Nanomaterials Challenges
   4.1. W. Kaysser: Structural Nanomaterials
   4.2. R. Feidenhans´l: New Phenomena related with Nanomaterials
   4.3. U. Steinsmo: Future Challenges in Nanocatalysis
   4.4. K. Carneiro: Nanostandardisation
5. Nanotechnology
   5.1. L. Schlapbach: GENNESYS: Industrial Groupings
   5.2. P. Fratzl: Biomaterials and Biotechnology
6. Nanoscience and Nanotechnology Initiatives in USA and Japan
   6.1. R. W. Siegel: Nanomaterials research in the USA
   6.2. H.Nakasawa: Nanomaterials research in Japan
7. Future Visions of European Synchrotron Radiation and Neutron Sources
   7.1. C. Vettier: GENNESYS: New Challenges for synchrotron radiation and neutron facilities
   7.2. N. Mårtensson
8. European Industry
   8.1. B. Barbier (LETI): GENNESYS: New opportunities for the nanoelectronics industry
   8.2. J. Rieger (BASF): GENNESYS: New potentials for the chemical industry
   8.3. A. Molenbroek (HALDOR TOPSOE): GENNESYS: New opportunities for catalysis
9. GENNESYS Organisation (P. Tindemans)
10. Closing Remarks (H. Schunck, BMBF)



7TH FEBRUARY 2005, PARIS

GENNESYS Presentation at the OECD Global Science Forum
Advanced analysis in nanospace: from fundamental research to new technologies (H. Dosch)

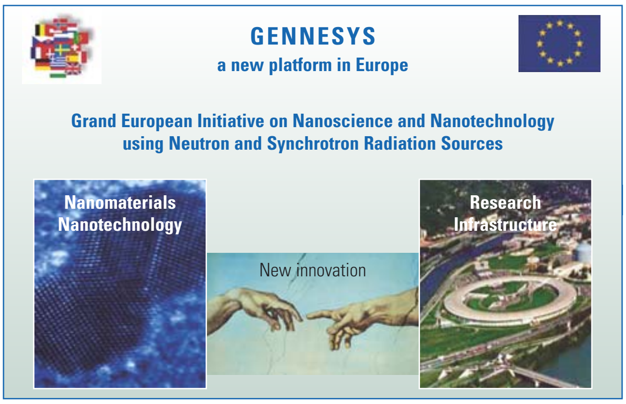
DEC 6–7 2005, NOTTINGHAM

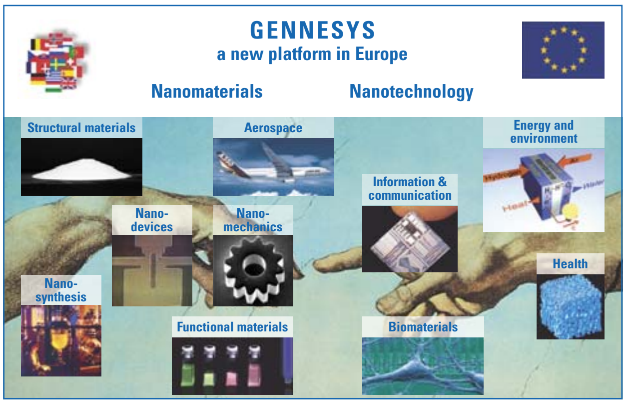
GENNESYS Presentation at 3rd European Conference on Research Infrastructures
European Commission workshop held in Nottingham during the 2005 British presidency of the EU
GENNESYS: A New Platform in Europe (W. Kaysser, GKSS)

CONCLUSIONS

- Breakthroughs in nanomaterials will create great potential for next-generation technologies.
- The large facilities will be an essential element in achieving this goal.
- If Europe strives for a leading position (in the world) in nanomaterials science and technology, the gap between materials communities in science and industry and the large facilities must be bridged. To this end, a scheme on the European level needs to be put in place.
- Nanosciences will offer great challenges to future innovations of large-scale facilities, for example:
  - In-situ observation in synthesis and industrial processing
  - Real-time resolution in sub-picoseconds for degradation mechanism nanomaterials – real environmental conditions (e.g. industrial)

In order to realise the above objectives, national and European operational networking mechanisms will be adopted. New mechanisms may have to be implemented, e.g. the creation of European Science/Technology Centres of Excellence in key areas.
A strategic document highlighting the research needs for the next decade will soon be issued by GENNESYS.





14. APPENDIX II: LIST OF ACRONYMS

A

ABWR	Advanced Boiling Water Reactor
AC	Alternating Current
ACARE	Advisory Council for Aerospace Research in Europe
AD	Arc Discharge
AES	Auger Electron Spectroscopy
AFM	Atomic Force Microscopy
AI	Amelogenesis Imperfecta
ALBA	Synchrotron Light Facility (Spain)
AML	Advanced Measurement Laboratory
ANKA	Angstromquelle Karlsruhe
APD	Avalanche Photo Diode
ARPES	Angle-Resolved Photo Emission Spectroscopy
ASAXS	Anomalous Small Angle X-ray Scattering
ASICs	Application Specific Integrated Circuits
ASTRID	Aarhus Storage Ring in Denmark
ATO	Antimony Tin Oxide
ATRP	Atom Transfer Radical Polymerisation

B

B(Gd)NCT	Boron (Gadolinium) Neutron Capture Therapy
BENSC	Berlin Neutron Scattering Center
BESSY	Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung
BMG	Bulk Metallic Glass
BNC	Budapest Neutron Centre
BOEL	Back End of Line
BSCCO	Bismuth, Strontium, Calcium, Copper, Oxide
BTL	Biomass to Liquid
BWR	Boiling Water Reactors

C

CAD/CAM	Computer-AidedDesign/Computer-Aided Manufacturing
CALTECH	California Institute of Technology
CANDU	Canada Deuterium Uranium
CBRN/E	Chemical, Biology, Radiologic, Nuclear/Explosive
CCD	Charge-Coupled Device
CCN	Cloud Condensation Nuclei
CCS	Carbon Capture and Sequestration
CD & LER	Critical Dimension and Line-Edge Roughness
CDI	Carbonyldiimidazole
CDS	Carbide Dispersion Strengthened (alloys)
CD-SAXS	Critical Dimension Small Angle X-ray Scattering
CEA	Commissariat à l'Énergie Atomique
CFRP	Nanoclay Carbon Fibre-Reinforced Plastics
CFTM	Computational Fourier Transform Moiré
CLOM	Confocal Scanning Microscope
CM	Cryogenic Melting
CMAS	Calcium Magnesium Aluminium Silicate
CMCs	Ceramic Matrix Composites
CMOS	Complementary Metal Oxide Semiconductor
CNRP	Carbon Nanotube Reinforced Polymers
CNT	Carbon Nanotube
COST	Concerted Action for Science and Technology
CPA	Coherent Potential Approximation
CPU	Central Processing Unit
CRT	Cathode Ray Tube
CTL	Coal-to-Liquids
CVC	Chemical Vapour Condensation
CVD	Chemical Vapour Deposition
CVS	Chemical Vapour Synthesis

D

DD	Dislocation Dynamics
DESY	Deutsches Electronen-Synchrotron
DFT	Density Functional Theory
DIC	Digital Image Correlation
DINS	Deep Inelastic Neutron Scattering
DLC	Diamond-Like Carbon
DLP	Digital Light Processor
DLS	Dynamic Light Scattering
DMFC	Direct Methanol Fuel Cell
DNA	Deoxyribo Nucleic Acid
DNS	Diffuse Neutron Scattering
DOE	Department of Energy
DORIS	Doppel-Ring Speicheranlage
DRAM	Dynamic Random Access Memories
DSC	Differential Scanning Calorimetry
DTA	Differential Thermal Analysis

E

E&P	Exploration and Production
EACRO	European Association of Contract Research Organisations
EB-PVD	Electron Beam Physical Vapour Deposition
EC	European Commission
ECNAT	European Centre of Excellence in Nanotribology
ED	Electrodynamics
EDOC	Electrochemical Deposition under Oxidising Conditions
EDX	Energy Dispersive X-ray Spectroscopy
EDXRD	Energy-Dispersive X-ray Diffraction
EELS	Electron Energy Loss Spectroscopy
EIRMA	European Industrial Research Management Association
EIT	European Institute of Technology
EM	Electron Microscope
EMA	Effective Medium Approximation
EMBL	European Molecular Biology Laboratory
EMEA	European Medicines Agency
EMI	Electromagnetic Interference
EOR	Enhanced Oil Recovery
EPD	Electrophoretic Deposition
EPI	Electrophoretic Impregnation
EPR	European Pressurised Reactor

ERA	European Research Area
ERC	European Research Council
ERL	Energy Recovery Linear
ERLs	Energy Recovery Linacs
ESD	Electrostatic Discharge
ESEM	Environmental Scanning Electron Microscope
ESF	European Science Foundation
ESFRI	European Strategy Forum for Research Infrastructure
ESI	Electron Spectroscopic Imaging
ESRF	European Synchrotron Radiation Facility
ETBE	Ethyl Tertiary Butyl Ether
ETFE	Ethylene Tetrafluoroethylene Copolymere
EUA	European University Association
EUV	Extreme Ultra-Violet
EUV-IL	Extreme UV Interference Lithography
EUVL	Extreme Ultra-Violet Lithography
EXAFS	Extended X-ray Absorption Fine Structure

F

FAME	Fatty Acid Methyl Esters
FAST/SPS	Field-Assisted Spark-Plasma Sintering
FDA	Food and Drug Administration
FE	Finite Element
FEL	Free Electron Laser
FEOL	Front-End-of-Line
FEP	Fluorinated Ethylene Propylene
FET	Field Effect Transistor
FGLM	Fine Grating Laser Moiré
FIB	Focused Ion Beam
FIB- SEM	Focused Ion Beam – Scanning Electron Microscope
FIR	Far-Infrared Spectroscopy
FLASH	Free Electron Laser in Hamburg
FM	Frequency Modulation
FOD	Foreign Object Damage
FRAM	Ferroelectric Random Access Memory
FRG	Forschungs Reaktor Geesthacht
FRM	Forschungs Reaktor München
FST	Fire, Smoke, Toxicity
FT-IR	Fourier Transform Infrared Spectroscopy

G

GFR	Gas-cooled Fast Reactor
GFRP	Glass Fibre-Reinforced Plastic
GGG	Gadolinium Gallium Garnet
GID	Grazing Incidence Diffraction
GISANS	Grazing Incidence Small-Angle Neutron Scattering
GISAXS	Grazing Incidence Small-Angle X-ray Scattering
GM	Genetically Modified
GMR	Giant Magneto Resistance
GNP	Gross National Product
GTL	Gas-to-Liquids

H

H/D	Hydrogen/Deuterium
HEX	High-Energy X-rays
HEXS	High-Energy X-ray Scattering
HF	High Frequency
HLW	High-Level Waste
HP	High Pressure
HPRM	Hydrogen Plasma Melting Reaction
HR	High Resolution
HREELS	High Resolution Electron Energy Loss Spectroscopy
HRTEM	High Resolution Transmission Electron Microscopy
HR-XPS	High Resolution X-ray Photoelectron Spectroscopy
HSP	Hybrid Sugar-Peptide
HSS	Hybrid Sugar-Synthetic
HT	High Temperature
HTC	High Temperature (superconductor)
HTP	High Throughput Platform
HV	High Voltage
HVOF	High Velocity Oxygen Fuel

I

IC	Integrated Circuit
ICS	Inverse Compton Scattering
IE	Industrial Ecology
IEA	International Energy Agency
IGC	Inert Gas Condensation
ILL	Institut Laue Langevin
INS	Inelastic Neutron Scattering
IPANEMA	Institut Photonique d'Analyse Non-destructive Européen des Matériaux Anciens
IR	Infrared
ISO	International Organisation for Standardisation
ITRS	International Technology Roadmap for Semiconductors
ITS	Inelastic Tunnelling Spectroscopy
IXS	Inelastic X-ray Scattering

J

JEEP	Joint Engineering, Environmental and Processing Beam line

L

LALLS	Low Angle Laser Light Scattering
LD	Laser Deposition
LDH	Layered Double Hydroxides
LDLM	Large Deformation Laser Moiré
LED	Light-Emitting Diode
LEED	Low-Energy Electron Diffraction
LFR	Lead-cooled Fast Reactor System
LIGA	Lithographie, Galvanofomung, and Abformung
LINAC	Linear Accelerators
LLB	Laboratoire Léon Brillouin
LSCM	Laser Scanning Confocal Microscopy

LSF Large-scale Scientific Facilities
LSI Laser Speckle Interferometry
LTC Low Temperature (superconductor)
LV-SEM Low-Voltage Scanning Electron Microscope
LWR Light Water Reactors

M

MBE Molecular Beam Epitaxy
MD Molecular Dynamics
MEMS Micro-Electromechanical Systems
MET Micro-Exposure Tool
MFM Magnetic Force Microscopy
MIB Metallic Intermediate Band
MIM Metal Insulator Metal
MMC Metal-Ceramic Nanostructured Matrix Composites
MMC's Metal Matrix Composites
MOKE Magneto-Optical Kerr Effect
mPILC Magnetised PILC
MPP Microwave Plasma Process
MPU Microprocessor Units
MRAM Magnetic Random Access Memory
MRI Magnetic Resonance Imaging
MSM Magnetic Shape Memory
MSR Molten Salt Reactor System

N

NBIC Nano Biology Information Cognition
ND Neutron Diffraction
NDS Nitrides Dispersion Strengthened (alloys)
NDT Nondestructive Testing
NEMS Nano-Electro Mechanical Systems
nFET Negative Channel Field Effect Transitor
Ni-MH Nickel-Metal Hydride
NIST National Institute of Standards and Technology (U.S.)
NITE Nano-Powder Infiltration and Transient Eutectoid
NMOS Negative Metal Oxide Semiconductor
NMP Nitroxide-Mediated Polymerisation
NMR Nuclear Magnetic Resonance
NR Neutron Reflectometry
NSE Neutron Spin Echo
nZVI Nanoscale Zero-Valent Iron

O

OA Organic Aerosol
OAM Open Access Mode
ODS Oxide Dispersion Strengthened
OLED Organic Light-Emitting Diode
OM Optical Microscopy
OMTA Optical Multichannel Transducer Array

P

PAH Polycyclic Aromatic Hydrocarbons
PALS Positron Annihilation Lifetime Spectroscopy
PC Photonic Crystal
PCN Polymer Clay Nanocomposites
PCRAM Phase Change Random Access Memory
PDF Partial Pair Distribution Functions
PEELS Parallel Detection Electron Energy Loss Spectroscopy
PEEM Photo-Electron Emission Microscopy
PEM Polymer Electrolyte Membrane
PES Photo Emission Spectroscopy
PETRA Positron-Elektron-Tandem-Ringanlage
pFET Positive Channel Field Effect Transistor
PILC Pillared Clay
PLD Pulsed Laser Deposition
PMCS Polymer-Matrix Composites
PMOS Positive Metal Oxide Semiconductor
PSC Polar Stratospheric Clouds
PSI Paul Scherrer Institute
PV Photo Voltaics
PVD Physical Vapour Deposition
PWR Pressurised Water Reactors
PYSZ Partially Stabilised Zirconia
PZT Lead Zirconium Titanate

Q

QD Quantum Dot
QED Quantum Electro Dynamics
QNS Quasielastic Neutron Scattering

R

R&D Research and Development
RAFT Reversible Addition Fragmentation Chain Transfer
RDF Radial Distribution Functions
REE Rare Earth Element
RF Radio Frequency
RFID Radio Frequency Identification
rhBMP-2 Recombinant Human Bone Morphogenetic Protein
RHEED Reflection High Energy Electron Diffraction
RID Reactor Institute Delft (Netherlands)
RIE Reactive Ion (plasma) Etching
RIXS Resonant Inelastic X-ray Spectroscopy
RME Rapeseed Methyl Ester
RN Radionuclides
RNA Ribonucleic Acid
RTM Resin Transfer Moulding
RXS Resonant X-ray Scattering

S

S/EXAFS Surface EXAFS
SALLS Small Angle Laser Light Scattering
SANS Small Angle Neutron Scattering
SAW Surface Acoustic Wave
SAXS Small Angle X-ray Scattering
SC Superconductor

SCL Supercooled Liquid
SCWR Supercritical Water-cooled Reactor System
SDS Sodium Dodecyl Sulphate
SEM Scanning Electron Microscopy
SEMPA Scanning Electron Microscopy With Polarisation Analysis
SERS Surface Enhanced Raman Spectroscopy
SET Single Electron Transistor
SFA Surface Force Apparatus
SFNF'S Superconductor/Ferromagnet/Non-magnet, Ferromagnet/Superconductor
SFR Sodium-cooled Fast Reactors
SFS Superconductor/Ferromagnet/Superconductor
SIMS Secondary Ion Mass Spectroscopy
SINQ Swiss Spallation Neutron Source
SiP System-in-Package
SLS Swiss Light Source
SMCs Sheet Moulding Compounds
SME Surface Modifying End
SME's Small and Medium-sized Enterprises
SNF Spent Nuclear Fuel
SNG Synthetic Natural Gas
SNOM Scanning Near-field Optical Microscopy
SNS Spallation Neutron Source
SOA Secondary Organic Aerosols
SoC System-on-Chip
SOFC Solid Oxide Fuel Cell
SOI Silicon on Insulator
SOLEIL Synchrotron SOLEIL
SPM Scanning Probe Microscope
SPR Surface Plasmon Resonance
SPS Spark Plasma Sintering
SQUID Superconducting Quantum Interference Device
SR Synchrotron Radiation
SR PEEM Synchrotron Radiation Photo-Electron Emission Microscopy
SRAM Static Random Access Memory
SRES Surface Roughness Evolution Spectroscopy
SRM's Standard Reference Materials
SRN Synchrotron Radiation & Neutron
SRS Synchrotron Radiation Source, Daresbury (UK)
SSRT Stereotactic Synchrotron Radiation Therapy
STI Shallow-Trench Isolation
STM Scanning Tunnelling Microscopy

T

TA Thermal Analysis
TBC Thermal Barrier Coating
TEM Transmission Electron Microscopy
TEP Thermopower
TMR Tunnel Magnetoresistance
TOF Time-of-Flight
TRL Technology Readiness Level

U

UFG Ultrafine Grained
UHV Ultrahigh Vacuum
UPS Ultraviolet Photoelectron Spectroscopy
USANS Ultrasmall Angle Neutron Scattering
USAXS Ultrasmall Angle X-ray Scattering
USF User Support Facilities
UV Ultraviolet
UVA Ultraviolet Radiation of Relatively Long Wavelengths
UVB Ultraviolet Radiation of Relatively Short Wavelengths

V

VHTR Very High Temperature Reactor
VOC Volatile Organic Carbon

W

WANS Wide Angle Neutron Scattering
WAXD Wide Angle X-ray Diffraction
WAXS Wide Angle X-ray Scattering
WER/RBMK Graphite Moderated Light Water Reactors
WMD Weapons of Mass Destruction

X

X/N X-ray/ Neutron
X/ND X-ray/ Neutron Diffraction
X/NR X-ray/ Neutron Radiation
XAFS X-ray Absorption Fine Structure
XANES X-ray Absorption Near Edge Spectroscopy
XAS X-ray Absorbtion Spectroscopy
XES X-ray Emission Spectroscopy
XFEL X-ray Free Electron Laser
XMCD X-ray Magnetic Circular Dichroism
XPCS X-ray Photon Correlation Spectroscopy
XPEEM X-ray Photoelectron Emission Microscopy
XPS X-ray Photo-electron Spectroscopy
XRD X-ray Diffraction
XRF X-ray Fluorescence
XSW X-ray Standing Wave

Y

YBCO Y-Ba-Cu-O Based Superconductor

15. KEY WORD INDEX