

# 9. MATERIALS SCIENCE AND BASIC RESEARCH IN EUROPE: CONCLUSIONS AND RECOMMENDATIONS

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This White Book reflects the vision of a diverse group of leading scientists in Europe concerning the future of materials science. Experts in the field are convinced that high-performance materials are the basis for all key technologies and, thus, the future of every modern society. There is also common agreement that the challenges concerning the increased complexity of high-tech materials and greater world-wide competition can only be met by well-organized, joint European Commission (EC) research programmes in basic materials science that ensure sustained financial support and the highest level of expertise. A number of recommendations for the European Commission authorities currently preparing the next Framework Programme have been formulated with the sole purpose of making this vision a reality. These recommendations are:

- Materials research in the EC should be given the same priority as biotechnology and informatics. Materials science plays a crucial role in the development and competitiveness of these and many other technologies, especially in the transport, chemical, energy, electronics, and aeronautical industries.
- The EC budget for basic science needs to be increased to a level comparable with that of Japan in order to remain competitive in the 21<sup>st</sup> Century, in particular with the Pacific region.
- European materials research programmes have to be coordinated to avoid unnecessary duplication between research groups in different Member States, to promote efficient use of resources, and to look for possible synergies.
- The basic research, development and evaluation of materials should fall under the jurisdiction of a European

materials science agency, modelled on the National Science Foundation (NSF) in the U.S. or the Swiss Science Agency, with the minimum amount of bureaucracy.

- The EC materials programme should span materials research and materials technology, with emphasis on long-term fundamental research.
- The fragmented nature of materials research in Europe needs to be replaced with a more efficient organizational structure. This could be achieved by establishing Centres of Excellence in Materials Science and Technology to coordinate European-wide research efforts.
- The number of interdisciplinary projects and education programmes has to be increased and greater interdisciplinary networking actively promoted in Europe.
- The EC should investigate plans for ensuring greater researcher mobility to make the most of Europe's diverse skill base and cultural heterogeneity for spawning new ideas. This should include the creation of a professional qualification for materials scientists and engineers (Eur-Mat) that is recognized throughout Europe.
- The EC should commence dialogue with non-scientists and other interest groups to find ways of countering the decreasing popularity of science in society. Steps should be taken to increase the profile of materials science through better education, science fairs, institute open days, summer schools, etc.
- Greater numbers of students enrolling in materials science and related courses at university are needed. This may be achieved by promoting greater awareness of the range of careers available, and also increasing salaries of academics working in these fields.

Priority research areas for European materials research should be:

### Materials discovery and design

To accelerate the design and exploration of new materials and novel phenomena and properties, priority should be given to the study of improved synthesis and processing, materials theory/modelling and advanced analytical techniques.

### Interdisciplinary research strategies

Completely new materials architectures and properties can be expected from the interplay between different types of materials systems, in particular from the design of devices made from inorganic and organic materials on the nano-scale. Interdisciplinary research between physicists, chemists and biologists should be supported and coordinated on a European level.

### Special materials with high innovation potential

Smart materials, biomaterials and nanomaterials will be

among the fastest growing areas of materials science over the next few decades, as will be materials for alternative energy sources, including high temperature and magnetic materials. Priority should also be given to materials that improve our management of the environment, natural resources and recycling. Such areas should become an important part of the EC's long term research plans and suitable funding should be made available to ensure Europe leads the way in each of them.

This White Book should be regularly updated to serve as a source of ideas for policy makers, and academic and industrial research directors. In the following sections, key aspects regarding the future of materials science, including technological trends and research priorities, are summarized and recommendations made. With a concerted effort from all European researchers, institutes and governments, Europe can succeed at the forefront of materials technology and enhance both her economic performance and the standards of living of her citizens.

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## 9.1. Materials Phenomena and Techniques

### 9.1.1. Materials Phenomena and Properties

Understanding, control and tailoring materials phenomena and properties on a microscopic level are key targets in materials science. By doing so we can develop new materials to meet technological needs, and optimize materials use to reduce wastage and pollution.

In the past, the primary task of materials scientists was to quantitatively characterize phenomena and develop modern theories to explain them. Today we have accumulated detailed knowledge of a large number of different electric, magnetic, optical, mechanical, and thermal phenomena described in terms of classical or quantum correlations in condensed matter (Fig. 9.1). Materials science beyond the year 2050 will be characterized by the control of materials phenomena on the nanometre length and femtosecond time scales. Several major targets exist for future analytical techniques, such as:

**Microstructural design:** The further improvement of our understanding and control of mechanical, thermal and chemical properties of multicomponent alloys, composite materials, materials with nano-sized components, and ceramics is needed in various key technologies. A major challenge here is the multiscale nature of many phenomena, which requires detailed understanding of how structures at different length scales interact and influence each other over different time scales. This will require considerable effort on various fronts, including modelling and microscopic analysis.

**The tailoring of phenomena** in a controlled and reproducible way using nanotechnological concepts: Since most materials phenomena are of a cooperative nature, they depend strongly upon the size of the system and are effected by the presence of surfaces and interfaces. This will allow tomorrow's materials scientists to modify, for example, the electric and magnetic response of artificial structures to the precise values desired. Materials science is an extremely diverse and multidisciplinary field that covers a wide range of novel phenomena, often with the potential for immediate applications.

**Small-scale phenomena:** The small-scale regime offers real opportunities for developing sustainable and environmentally friendly materials that meet tomorrow's technological needs. Colloidal systems and biomimetic strategies are two examples of an array of new concepts that will

allow us to design small-scale systems with greater multifunctionality. The size dependence of properties such as hardness and superplasticity will give rise to new mechanical phenomena ("smaller is tougher") and new thermodynamic behaviour that will have enormous impact on future technologies.

**Dynamic response of systems over very short time scales:** Understanding and (in future) controlling ultra-fast processes in materials is currently of great scientific and technological interest. It has recently become possible to probe dynamical phenomena in materials on ultra-short time scales down to sub-picoseconds (see Sect. 9.4). The study of ultra-fast structural relaxation phenomena will improve our understanding of phase transformations and structure formation. Rapid switching of magnetic domains in artificial structures will be used in tomorrow's information technology. These are just two examples of this important emerging field. Strong input and guidance from materials analysis and materials modelling will also be indispensable.

**The study of phenomena under extreme conditions:** The behaviour of materials under high pressures, high temperatures, high magnetic and electric fields is still poorly understood. Such studies are complicated and require expensive and sophisticated instrumentation, but have become possible with the availability of equipment for producing extreme external fields.

**Dynamic and dissipative phenomena at surfaces and interfaces:** With further developments in nanotechnology, the need to understand dissipative phenomena, lubrication and friction on an atomic level and in systems confined to the nano-scale will increase rapidly. These studies will ultimately lead to *in situ* studies of atomic friction on ultra-short time scales. Microscopic insight into the structural changes that take place during corrosion and catalytic and electrolytic reactions are of fundamental importance for the active control of these chemical reactions, in which both molecular reactivity and surface morphology play a role. It has become clear during the last few years that the ultimate understanding of these (also technologically important) physicochemical phenomena requires microscopic information of the dynamic behaviour of both electrons and nuclei. This information can only be obtained using spectroscopy-microscopy and spectroscopy-diffraction techniques in real time (see Sect. 9.1.4).

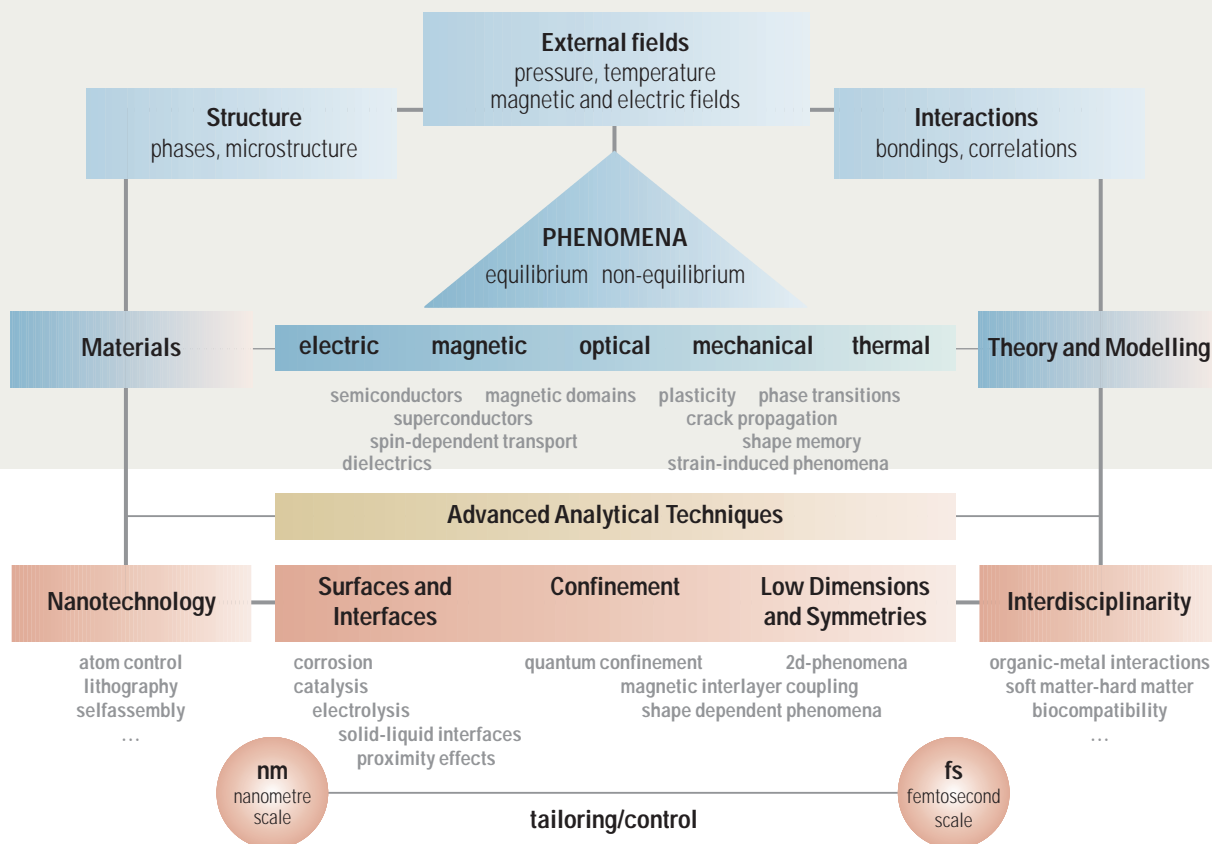


Fig. 9.1. Materials phenomena: interrelation between materials, modelling, analysis and future trends.

### 9.1.2. Synthesis and Processing

Synthesis and processing are fundamental to materials R&D, with new or improved methods usually leading to new materials or superior properties. Synthesis and processing are also responsible for the production of high quality, low cost products throughout the manufacturing industry. The main areas of innovation in synthesis and processing are:

- increased control over complexity, composition, structure, and function;
- water-based solution chemistry for low-cost, environmentally benign synthesis;
- rapid forming for use in combinatorial chemistry and the search for new materials;
- tailoring of materials at all length scales, from the atomic to macro-scales;
- computer modelling of complex phenomena to improve understanding and control;
- thin films and coatings for improved properties and component lifetimes;

- supercritical fluid chemistry for preparing new materials and nanomaterials as oxides, nitrides, metals with controlled both shape and size, continuously from micronic to nano-scales.

Basic research is still needed in the areas of crystal growth, vapor deposition, sintering, phase transformation, and rheology to better understand how they affect and can be controlled during synthesis and processing. Fig. 9.2 outlines the main areas of development for these techniques in the future.

Recommendations for priority research areas in materials synthesis and processing are:

#### Miniaturization

Miniaturization will be one of the most important goals of materials synthesis and processing in the near future. New processing technologies will be required to create all kinds of materials on ever smaller length scales. These techniques will enable manipulation of individual nanostructured units and atoms, and should be amenable to auto-

mation and parallel processing so that combinatorial approaches can be used to discover and optimize materials.

### Biomimetics and biomaterials

The field of biomimetics is one of the most challenging fields for synthesis and processing of organic materials. In medicine, new biomaterials are urgently needed for a variety of uses (e.g., implants, biosensors). It is still not clear, however, how such materials can be synthesized in a well-controlled and reliable fashion, since the knowledge on biomineralization and other natural synthesis processes is still in its infancy.

### Complex structures with building blocks/assemblies

Complex, functional structures or assemblies are constructed from building blocks on both the nano- and the meso-scales. Structure development is driven by self-organization. The confinement of highly dispersed Nano Building Blocks (NBBs) in hybrid or inorganic matrices or the organization of NBBs on textured substrates could provide larger concentrations of active dots, better defined systems, avoid coalescence into larger ill-defined aggregates while keeping or enhancing specific magnetic, optical, electrochemical, chemical and catalytic properties into the nanostructured hybrid materials.

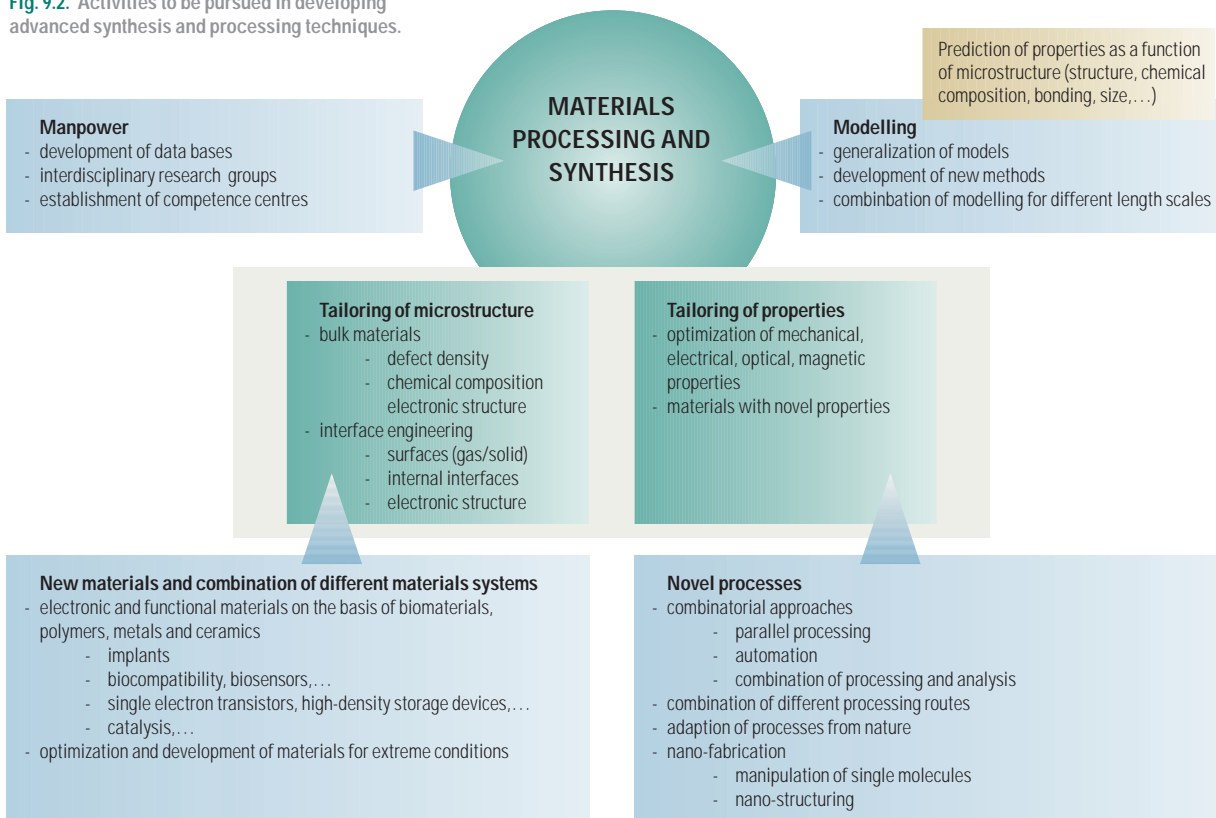
### Interface engineering

Interface engineering is an increasingly important means of improving and optimizing all kinds of materials from metals, ceramics and superconductors to bio- and smart materials. This field includes processing and tailoring of surfaces and interfaces for special applications like microelectronics and catalysis. Miniaturization results in interfaces becoming one of the dominant defects in a material; in some cases, these interfaces are necessary to obtain specific phenomena. Interface engineering is therefore a vital component of many future technologies.

### Modelling and automation of materials synthesis and processing

Trial-and-error experimental approaches are inefficient ways of designing and discovering materials. Modelling of synthesis and processing is a powerful tool for deciding which directions to pursue, and which are non-feasible or uneconomic. These techniques have proven valuable for many years in traditional fields, like steel processing. Although urgently needed, modelling of nano- and biomaterials processing has only just begun. Automated processing must be sufficiently accurate if it is to be used for nano-fabrication.

**Fig. 9.2.** Activities to be pursued in developing advanced synthesis and processing techniques.



### 9.1.3. Advanced Analytical Techniques

Progress in materials science is intimately related to achievements in the development of dedicated analytical techniques which enable us to examine the atomic and electronic structure of materials on the nanometre level and to unravel and quantitatively analyze condensed matter phenomena and processes. The current and future roles of modern techniques in the analysis of materials are summarized in Fig. 9.3.

Future targets in the design and processing of new materials, and monitoring and control of new phenomena and properties, are the generic driving forces for the development of new concepts and new techniques in diffraction, microscopy and spectroscopy. The highest possible resolutions, greatest sensitivities, and ultimate detection limits are the chief goals of this field, along with performing non-destructive and in situ analysis. One consequence of developments in this area will be that the traditional boundaries between the three major analytical methods (diffraction, microscopy, spectroscopy) will gradually disappear.

One possible scenario for how this key field of materials science can be organized in Europe is shown in Fig. 9.4. The following challenges in advanced analytical techniques will need to be met in the next decades:

#### High resolution microscopy

To obtain local, non-averaged structural information about inhomogeneous materials and structures, improved instrument resolutions will be needed to access smaller spatial domains, e.g.,

- sub-Å and sub-eV resolution in high resolution electron microscopy,
- 10 nm spatial resolution in X-ray microscopy.

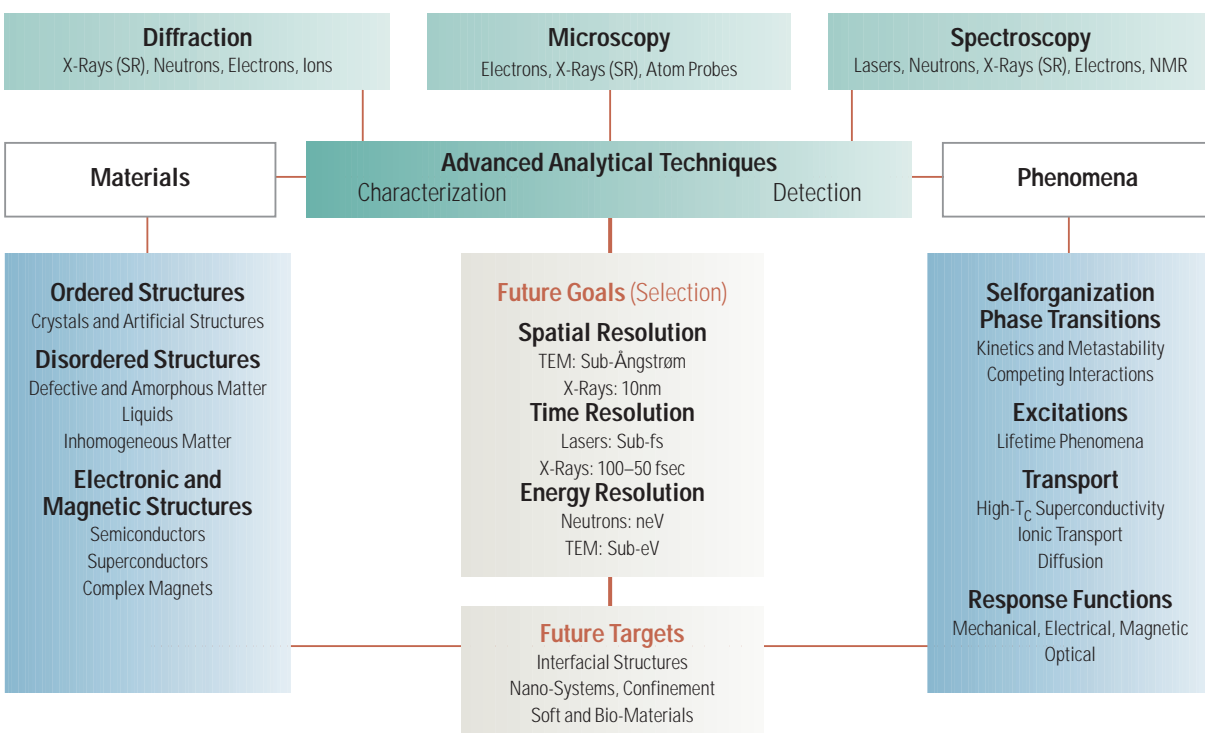
#### Real time characterization of materials and phenomena on femtosecond time-scales

The ultimate goal of this endeavour is to observe atomic motion in materials, particularly during chemical reactions and biological processes, directly. The same techniques could be used to control short-time relaxations of electrons and atoms during materials processing (e.g., modifying materials by ion beams). Quantifiable objectives include:

- 1 fs time resolution in laser spectroscopy
- 10 fs time resolution in X-ray diffraction

Achieving these ambitious goals, and thereby providing revolutionary insights into materials, will require new and expensive equipment and facilities, e.g., free-electron X-ray lasers. Such large-scale facilities can only be built and operated on a European level with strong commitment from Member States.

Fig. 9.3. The role of advanced analytical techniques for materials science, including future goals and targets.



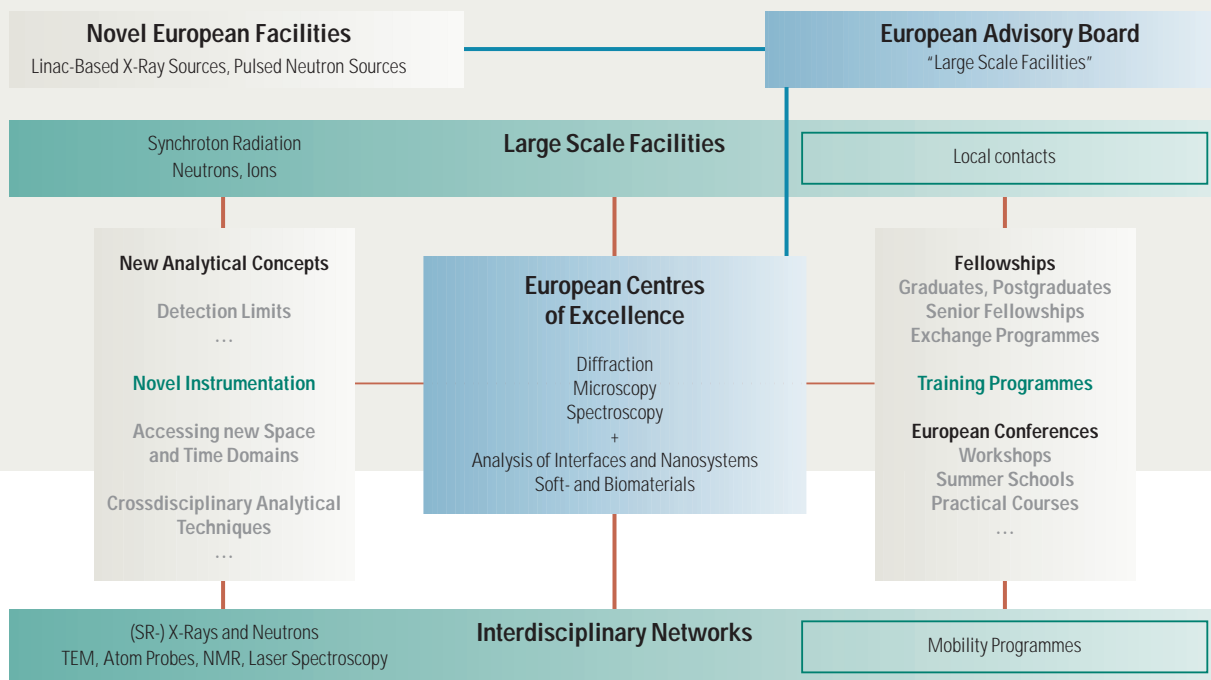


Fig. 9.4. European action plan for advanced analytical techniques.

### Efficient use of European large-scale facilities and modern techniques in materials analysis

New concepts in analysis are often developed by solid state physicists in dedicated laboratories or large-scale facilities with little or no contact with the materials scientists who could apply new techniques to the solution of "real world" problems. The efficient transfer of new ideas and breakthroughs in diffraction, microscopy and spectroscopy to the materials science community needs to be promoted by holding cross-disciplinary workshops and training courses. The institutes housing state-of-the-art facilities should also provide professional assistance to outside parties and act as "local contacts" with developers of new techniques.

### Creation of analytical networks and centres of excellence

The full potential of current and future analytical methods and apparatus can best be exploited if networks and centres of excellence are created which manage world-class facilities and provide high quality research and training opportunities.

#### 9.1.4. Materials Theory and Modelling

Computational materials science and engineering provide powerful tools for:

- prediction of novel structural and functional materials, e.g., nanomaterials,
- optimization of complex materials/design solutions

- simulation of materials synthesis, processing, microstructures and properties,
- development of history-dependent and of scale-bridging multi-scale simulation concepts,
- integration of electronic and atomic level as well as continuum scale approaches,
- studying phenomena that are not easily accessible by experiment,
- solving cost and time constraints for materials development and application.

A large number of computer modelling techniques are available for studying all kinds of materials and their behaviour from the quantum and atomic levels to microstructural and macroscopic levels over various time spans. Materials modelling will play an increasingly important role in materials design and the understanding of both fundamental and complex processes in all materials. The major themes for materials theory and materials modelling to be pursued within the EC over the next ten years are summarized in Fig. 9.5.

The following recommendations are made for ensuring Europe remains at the forefront of computational modelling of materials:

- Supercomputer facilities need to be installed or upgraded at more sites for large-scale simulations of fundamental materials processes and phenomena, e.g., sintering, crack propagation, catalysis.

- Interdisciplinary teams are needed to develop robust software and examine complex phenomena and materials.
- Computer laboratories in materials science departments need to be expanded and upgraded to include the latest PCs, workstations and simulation software tools.
- Training courses in materials modelling should be held regularly throughout Europe for students, academic and industrial researchers
- Networks for materials modelling are needed to aid long-term, large-scale simulation projects.
- Development of multi-scale modelling techniques should be given greater priority. This could be done by organizing collaborative projects between groups specialising in different simulation methods and length/time-scales.
- Collaboration between industry and academia in the development of simulation methods should be promoted.

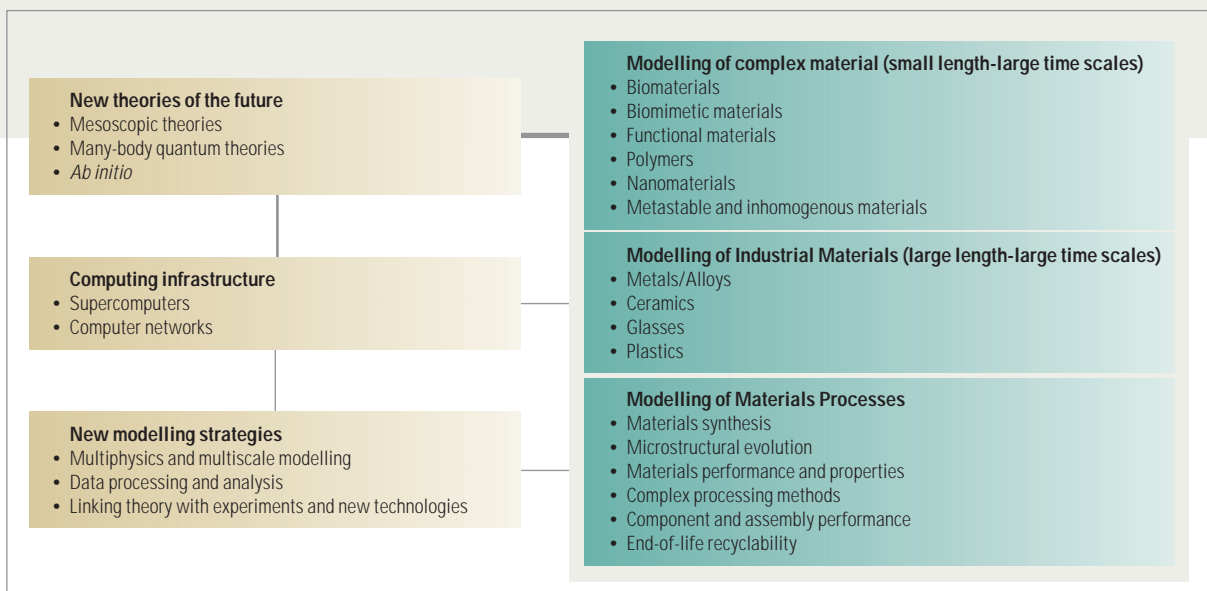


Fig. 9.5. Research priorities for materials modelling over the next decade.

## 9.2. Materials Systems

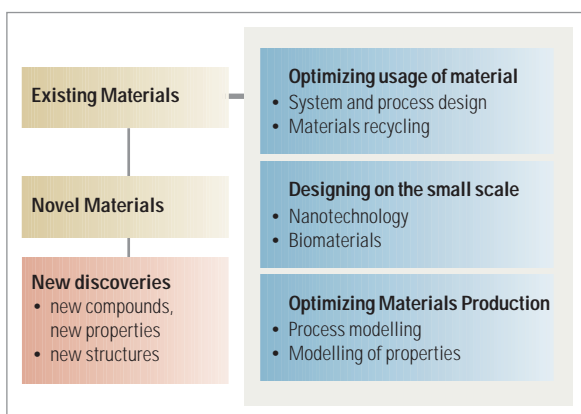


Fig. 9.6. Overall strategies for improvement of advanced materials into the 21<sup>st</sup> Century.

Materials can be divided into two broad groups; inorganic and organic materials. Inorganic materials are composed of non-carbon-based matter such as metals, ceramics and metalloids (e.g. silicon and germanium). Organic materials are based on carbon compounds, and include both living tissue and synthetic polymers. Materials can also be divided according to their properties or main applications, e.g., semiconductors, nanomaterials and catalytic materials. Technological progress in materials science can be brought about by modifying and improving existing materials or by developing novel materials resulting from new discoveries. These concepts are outlined in Fig. 9.6.

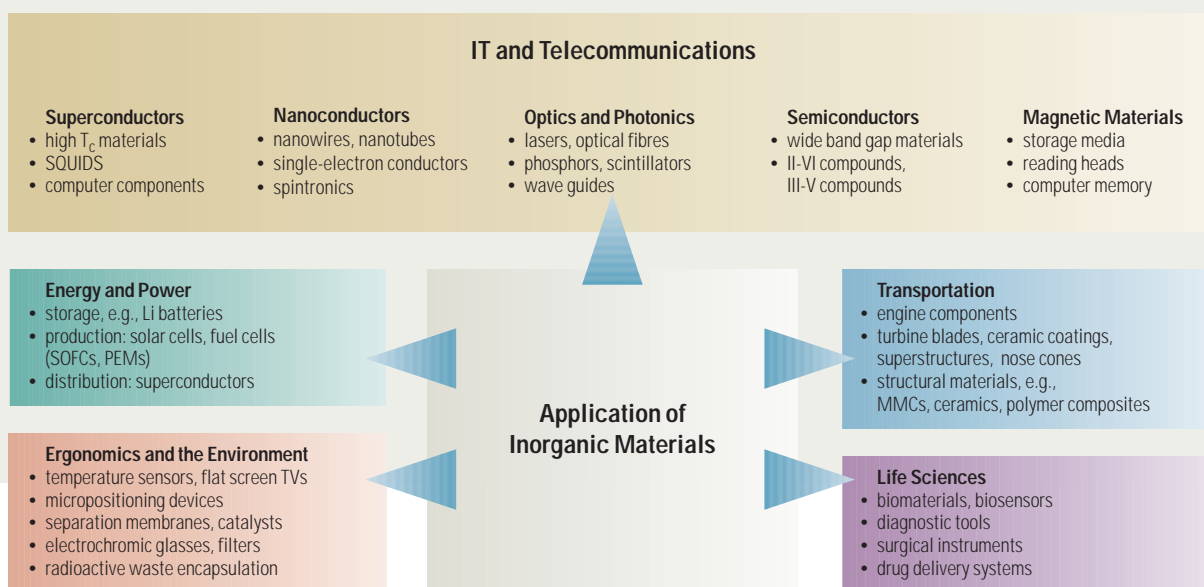


Fig. 9.7. The diversity and range of applications of inorganic materials.

### 9.2.1. Inorganic Materials

Research into advanced inorganic materials over the next ten years will reap benefits for five important sectors of the economy (Fig. 9.7). In all cases, basic research will be directed towards developing new synthesis methods allowing greater control over structure formation and smaller scale components. Research should also be directed at discovering new materials and compositions, structures and phenomena that will spawn new technologies, and revolutionize the way we manufacture goods, conduct business and spend our leisure time.

#### (a) Metallic materials

Metals and their alloys have the potential for further large improvements in properties and performance during the 21<sup>st</sup> Century. Due to their high stiffness, ease of forming, strength over a wide range of temperatures and, most importantly, their reliability, metals are the materials of choice for many engineering applications. They also often serve as the main phase in composites and adaptive systems because of their attractive properties. They range from low-cost bulk materials used in civil engineering to advanced, high added value materials tailored at the atomic level. The need to improve their corrosion resistance and their potential for recycling are important reasons for maintaining a high level of scientific, technical and industrial R&D in this field.

The basic scientific challenges lie particularly in pursuing fundamental and long-term oriented research in this field that is aimed at the development of well-tailored structures.

Major challenges lie in the development of lightweight structural materials, self-organizing microstructures, failure-tolerant materials systems and smart materials.

Metallic materials can be divided into four categories according to their present and future impact on economic and industrial activities, as summarized in Fig. 9.8. Important areas of metals research for the future include:

#### • Microstructural design of structural metals, alloys and their composites

Much remains to be understood concerning the microstructural design and optimization of multiphase metallic materials, which represent a large fraction of engineering structural materials. The corrosion and heat resistance of steels could be improved by better microstructural control, particularly at interfaces. Metal matrix composites also lend themselves to the systematic exploration of variations in multiphase metallic microstructures. Other important objectives include developing high strength-to-weight ratio structural materials, self-organising microstructures, failure-tolerant materials systems and smart materials.

#### • The physics of plasticity and damage

Better understanding is needed of the complex phenomena involved in deformation and fracture of metals, alloys, and metallic composites. New techniques for modelling the micromechanical behavior of materials that incorporate substructural phenomena (i.e., dislocations, boundaries, interfaces, and microvoids) coupled with focused experimental work should achieve this.

### • Complex metallurgy

Understanding of phase transformations and microstructural development in multicomponent alloys (e.g., superalloys and tool steels) has vastly improved with the advent of computer codes such as ThermoCalc: This research needs to be pursued further for (i) improved understanding of the fundamentals of the thermodynamics and kinetics of phase transformations, (ii) improved understanding of microstructure/property relations of each component from the atomic to macro-scales.

### • Liquid/solid processes

Many materials processes involve the coexistence of a liquid with a solid, e.g., liquid phase sintering, rheo/thixo-casting, and many composite fabrication processes. The physics of such processes have much in common, including the influence of capillarity, and fluid flow in the presence of fine-scaled solids. Progress in understanding and modelling these phenomena would provide significant benefits in terms of reduced costs and higher quality for many materials classes (composites, ceramics, metals).

the U.S. and Germany over the past ten years. Key challenges in this area are to lower the cost of processing, as current FGMs are generally uneconomical.

### • Novel metallic materials and systems

Unconventional combinations of different metals, microstructures and properties that have not yet been investigated could yield unexpected and useful materials. Novel synthesis and processing techniques should be used to explore these potential “goldmines”. Metals research should become more interdisciplinary, with metallurgists working closer with physicists, engineers, chemists and biologists to come up with new multimaterial systems.

### (b) Ceramic materials

A wide range of advanced ceramics are being developed for future applications such as environmental sensors, electronic components, turbine blades and fuel cells. Improved processing and quality control will enable structural ceramics to be used in niche areas such as aeronautics, space flight and power generation. The distinction between structural and functional ceramics will become blurred as smart materials, nanoceramics and bioceramics are developed.

The main directions which ceramics research will take in the future are summarized in Fig. 9.9. New design concepts such as biomimicry, hyper-organization, complex composite architecture and nanotechnology, combined with the increased understanding and predictive power provided by computer modelling, mean that advanced ceramics have a bright future. Challenges and foreseeable trends for ceramics research in Europe include:

**Fabricating new architectures via microstructural control and new processing routes.** The challenge is to create new classes of materials exhibiting previously unimagined properties by controlling the structure at the nano-level and using low cost and environmentally benign synthesis routes.

**Integration of ceramics with other materials.** In the future, ceramics will be combined with other conventional materials systems, both inorganic and organic, to provide greater functionality and reliability. These “smart” composites will be used in both structural and functional applications, far beyond the capabilities of most materials currently being used.

**Nanotechnology and miniaturization.** Investigation and exploitation of effects occurring at the meso- and nano-scales will become increasingly important over the next decade. Decreasing the size of ceramic components and their constituent grains can be expected to reveal a whole range of novel unexpected phenomena that can be put to use (e.g., as sensors or biomaterials).

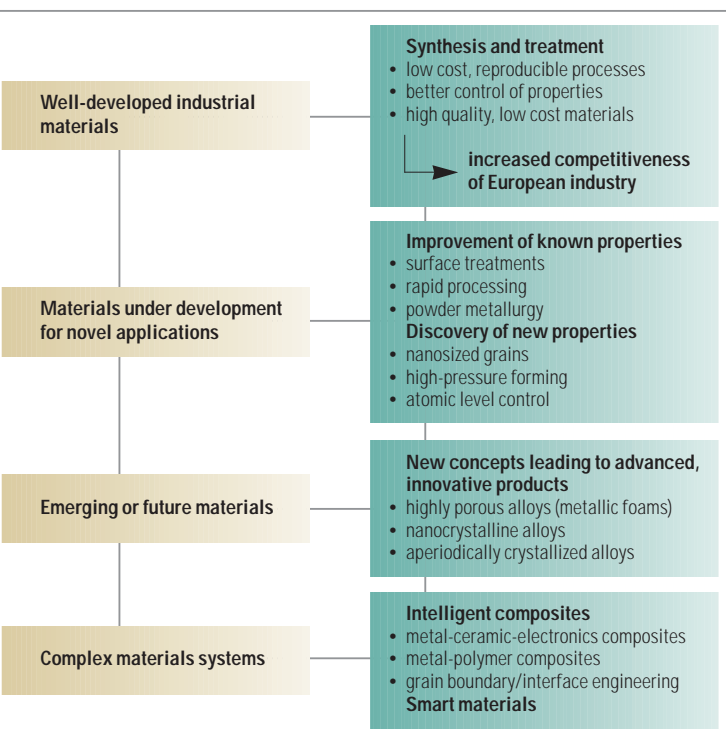


Fig. 9.8. Short-, medium-, and long-term research directions for metallic materials.

### • Functionally graded materials

Many structures require materials whose properties vary from one point to another. This leads to the concept of “functionally graded materials” (FGM), which have been the focus of several national research projects in Japan,

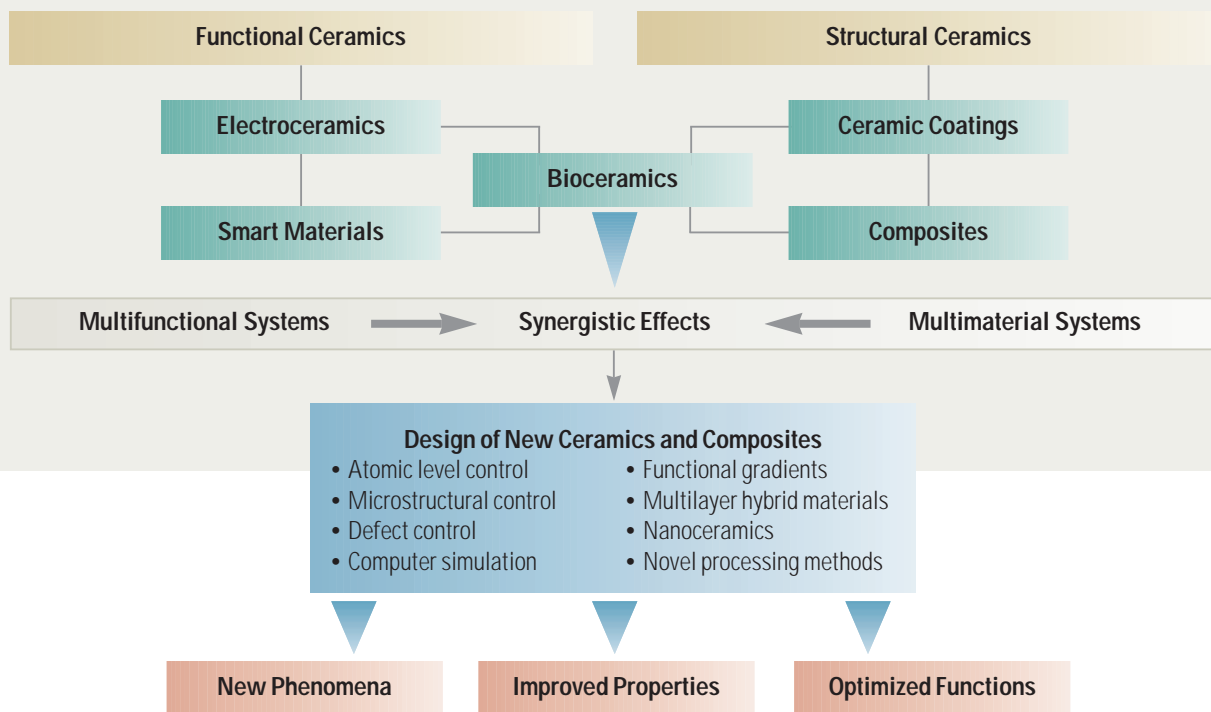


Fig. 9.9. Future advanced ceramics, including design concepts and goals.

**Increasing functionality of ceramic materials.** A whole range of new compounds and ceramic materials are being discovered with unusual properties that can be used in applications such as electronics, photonics, lasers, recording media, sonar, sensors, displays, batteries, infrared detectors. Intense effort is needed if Europe is to reap the rewards from this rich area of research.

Important recommendations for promoting ceramics research in Europe are:

**Greater uptake of advanced ceramics by industry**

Industry should be actively encouraged to incorporate the latest advanced ceramics into their products; although initial outlay can be greater, ceramics are generally longer-lasting, lighter weight and more heat-tolerant than alternative materials, so that greater savings are made in the long run. Ceramics also can provide more functionalities than cheaper, high volume materials.

**New initiatives in ceramic science**

The EC should fund new European-wide initiatives to develop advanced ceramic materials, especially ceramic matrix composites, bio- and electroceramics. Funding should be raised to a level comparable to that in Japan, which currently leads in the development and uptake of ceramic technology. These initiatives should include substantial industrial participation to ensure a critical mass of

researchers and availability of the latest equipment in this high-investment, high-returns field.

**Establishment of a European ceramics institute**

A European institute dedicated to advanced ceramics and covering the whole spectrum of these materials, including interdisciplinary areas such as bioceramics and nanoceramics, would greatly aid uptake of ceramics technology by smaller companies, as well as promote standardization of property measurement, materials quality, and European-wide collaboration.

**(c) Amorphous solids - glasses**

Long term research into the innovation of new vitreous materials merits special encouragement. This includes the discovery of brand new glass families by the control of subtle interactions among complicated sets of atoms, as well as the mastery of industrial compositions from a chemical bonding point of view. Huge efforts should be made in the understanding of the glass formation mechanisms and the modelling of glass structures.

**(d) Structural composite materials**

Composites offer the possibility of creating materials with superior properties or improved functionality by combining two or more disparate materials to form a single materials system. The main types of composites currently being investigated include polymer composites, metal matrix

composites and ceramic matrix composites. In the future we can expect to see an increasing use of biological materials in composites, particularly as research into biomimetic materials takes off and nature's secrets for producing ultra-hard but tough materials from the atomic level are revealed.

The main areas of future composites research should be:

- Smart composites incorporating sensors and actuators,
- Interface studies, particularly of delamination and internal friction;
- Computer modelling of complex architectures and shapes;
- Metal matrix, ceramic matrix and polymer matrix composites engineered on the nano-scale for use in different temperature regimes and exhibiting unique and superior properties;
- Development of new systems, e.g., aluminium-based alloys reinforced with silicon carbide and alumina particles, whiskers or fibres.

One of the greatest challenges for researchers is to understand the many complex interactions between the components of these materials. This requires a systematic approach to understanding, design and production. The creation of a Centre of Excellence for Structural Composites would provide for an integrated multipartner approach to elucidating the fundamentals of processing, design, optimization, and industrial implementation. This would advance the technology significantly and strengthen Europe's position in the field, in which it currently lags significantly behind North America. Transportation, electronic packaging, power transmission, aerospace, and

sports technology, to name presently established application areas, would all benefit from improvements in this field.

## 9.2.2. Organic, Bio- and Biomimetic Materials

### (a) Polymeric materials

The field of polymeric materials is broad and extends from basic synthetic chemistry to process engineering. Research has traditionally been pursued in the laboratories of large chemical corporations and chemistry or chemical engineering departments of universities and research institutes. In the last few years a grown interest has emerged in combining knowledge from polymer science and other disciplines. Therefore the potential for creating new and innovative materials is enormous.

Basic research is still needed in many areas of polymer science. Model polymeric materials (low molecular, compositional and structural heterogeneity) are very important in order to understand the basics of structure-properties relationships. Priority research topics in polymer based materials are listed below and summarized in Fig. 9.10.

#### New synthesis methods:

- New mechanisms of polymerization, e.g., catalytic, enzymatic and free radical polymerization in dispersed media (emulsions, miniemulsions, etc) and under supercritical conditions
- Environmentally friendly methods using water as a solvent

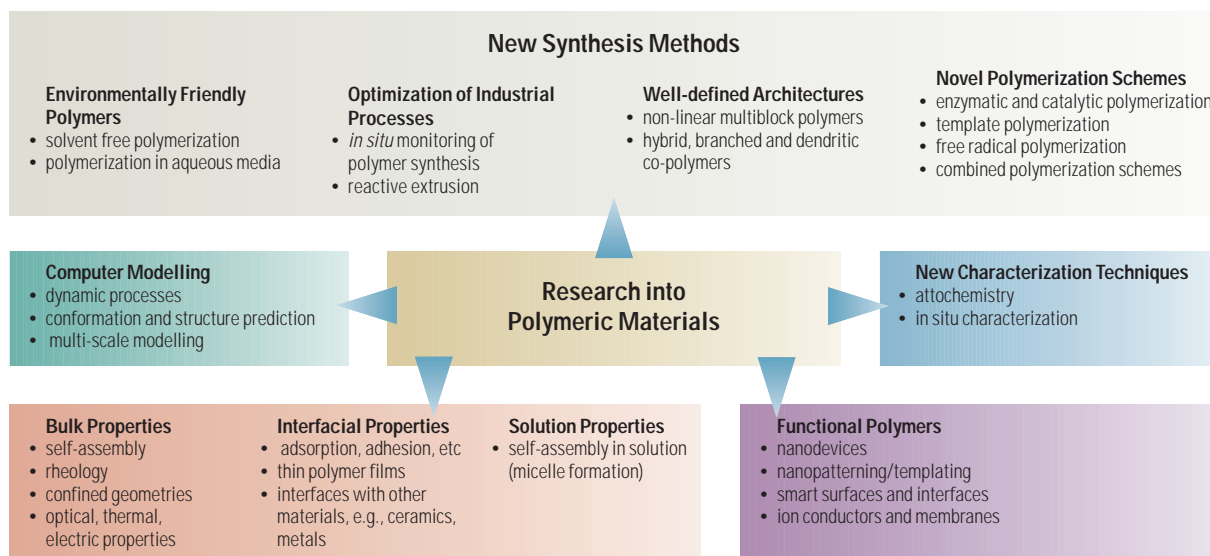


Fig. 9.10. Future research directions for polymeric materials.



- Nanopatterning via block copolymer self-assembly
- Combining of polymerization methods or transforming of one active centre to another
- Selective solubilization of low molecular weight compounds
- High purity synthesis

**Novel architectures and materials combinations:**

- Composite materials for greater strength and functionality
- Behavior at polymer interfaces
- Nanostructured materials based on polymers

**Functional polymers:**

- Polymers for optics and electronics, e.g. light emitting diodes, displays, sensors, batteries
- Membranes for fuel cells and batteries
- Polymers for biomedical applications (see b) below)
- High performance polymers (polyimides, fluoropolymers, etc.)
- Organic-inorganic hybrid structures
- Smart materials for sensing and responding to environmental changes

**Structure-property relationships**

- Computer modelling from atomic to macro-scales
- Structural organization and design at the atomic/nano-level
- Transport phenomena in ion-conducting and gas filtration membranes
- High speed analytical techniques

**(b) Bio- and biomimetic materials**

Biomaterials is a rapidly growing field of materials research that has important implications for the quality of life of Europe's ageing populations. The main research priorities are:

- Understanding of the fundamental mechanisms of biomaterial-cell interactions and identification of the quantifiable relationships between a material's surface characteristics and cell behaviour.
- Development of smart biomaterials that are able to sense tissue responses and release biological signals accordingly.
- Optimization of bone-bonding systems that can reliably and practically achieve stable fixation of prostheses to bone.
- Optimization of the architecture and microstructure of synthetic scaffolds to act as vehicles for three dimensional tissue regeneration.
- Development of systems that facilitate localized delivery of genes to diseased tissue.

Closely related to biomaterials are the biomimetics; these materials are synthesized by copying mechanisms and processes observed in Nature to provide optimal structures and properties. Biomimetics are used not only for medical purposes, but as structural, smart and functional materials also. Future research directions for both these fields are summarized in Fig. 9.11.

Europe is currently falling behind other regions in biomaterials research despite having the expertise and know-how. The strength of U.S. industry and size of its market is drawing many companies and researchers overseas. To remedy this situation, it is recommended that

- a database of implants, etc, be created to follow patient recovery over the long term.
- biomaterials be recognized as a legitimate field of research, e.g., by providing professorships, establishing university schools/departments.

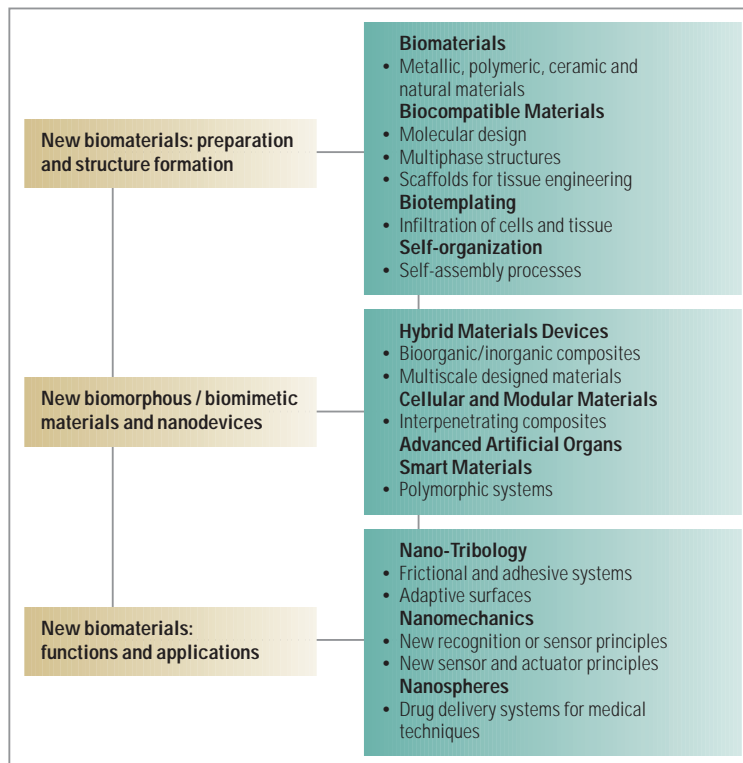


Fig. 9.11. Future research directions for bio- and biomimetic materials over the next decade.

- the EC convene multidisciplinary teams of experts to coordinate research efforts within the EU, and provide them with a boost in funding to establish biomaterials research centres specialising in different areas such as cardiovascular surgery, orthopaedics, ophthalmology.

- protocols for discussing various ethical issues surrounding the development and use of biomaterials be established-regulatory bodies are needed to oversee research, particularly when patient trials are involved.

### 9.2.3. Nanomaterials

Almost all future materials science will be based on nanotechnological concepts. Materials will be able to be assembled layer-by-layer or even atom-by-atom to generate new atomic arrangements with completely new properties. Nanomaterials are designed (and are used) today in a variety of forms, such as nanopowders, colloids, thin films and coatings, multilayers and laterally structured systems (from nanostripes and nanodots in semiconductor research to nanopore filters made from polymers). We are already today able to connect semiconducting materials with magnetic, superconducting, organic and even biological materials with nanometre control. Nanoscale materials science is governed by three main phenomena: **confinement, proximity and organization**. The interplay of these three phenomena creates rich new areas for uncovering novel materials behaviour.

Nanotechnology promises to revolutionize the way we live and work, from manufacturing and medicine to computing and communications. Many new and clever combinations of materials, molecules, atoms and ions will emerge

over the next few decades that display unusual and unexpected behaviour, thus allowing the development of tomorrow's devices and applications.

The confinement of materials to length scales below those producing ordinary macroscopic behaviour results in new spin and charge ground states, new electric and magnetic polarization textures, and new dynamics for polarization reversal and charge transport. Exchange of spin, charge, strain, electromagnetic fields, or matter across interfaces leads to novel proximity effects that profoundly affect the properties of neighbouring materials. These confinement and proximity effects can be precisely controlled through nanoscale organization, where the properties of hybrid materials are tuned by adjusting the feature sizes of the constituent materials. Fig. 9.12 summarizes key areas of research and applications in this field.

Future challenges in the science of nanomaterials:

- Nanoparticles, quantum structures, self-assembly materials and nanobiomimetics demand priority attention in the near future.
- Do we know all possible mechanisms which lead to self-organized structures?
- Is it possible to stabilize at room temperature (STM-manipulated) structures consisting only of a few atoms?
- Possibilities of designing nanostructures using organic components (organic FETs, organic light-emitting devices, etc.) and nano-sized magnetic domains that allow high density data storage, exhibit tailored hysteresis

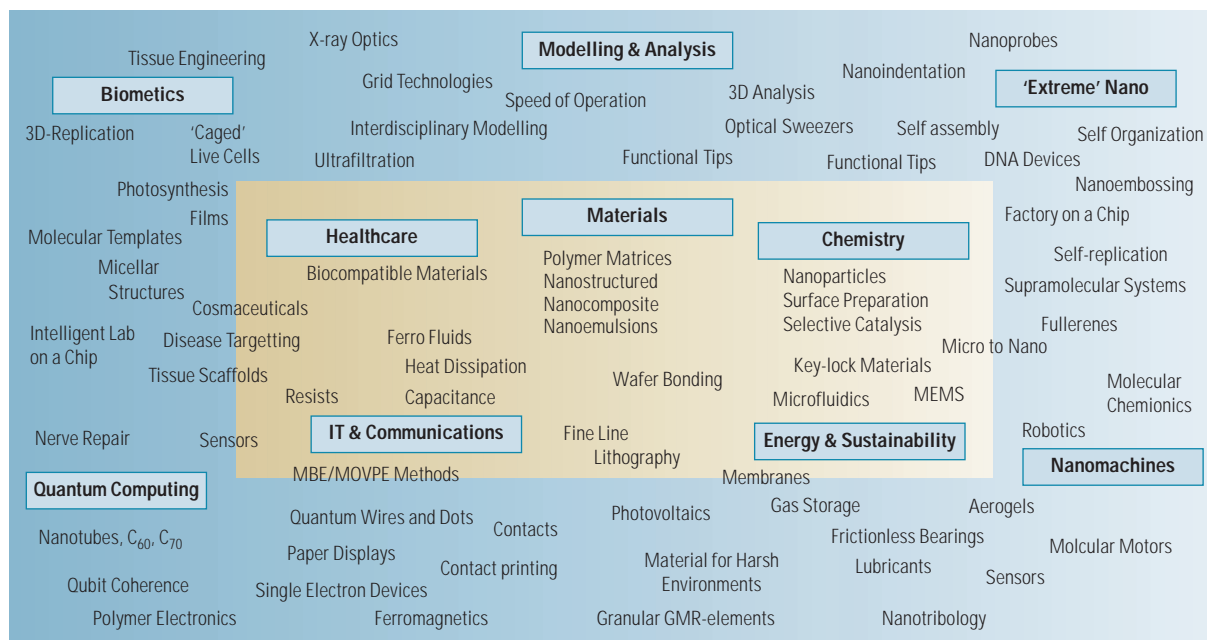


Fig. 9.12. A roadmap for nanomaterials research and applications in Europe.

0-5 years

>5 years

loops and can be switched at the highest speeds, need to be explored further.

- Further progress in spintronics depends on basic experimental and theoretical studies of ferromagnetic-semiconducting interfaces and nanostructures which preserve the electronic polarization.
- It is also important to realise that current technologies, particularly those based on semiconductor materials, are reaching their physical limits. Strong and coordinated basic research programmes are necessary now to come up with new ideas for overcoming these barriers.
- Nanotechnology is an essential part of any such strategy. For example, nanomaterials may open the door to new devices in the fields of quantum computing, quantum electronics, photonics and magnetics.
- Formation of quantum dots and wires of uniform size and distribution will be a demanding research field, as will be the fabrication of materials architectures and functioning circuits from these components to form useful devices.

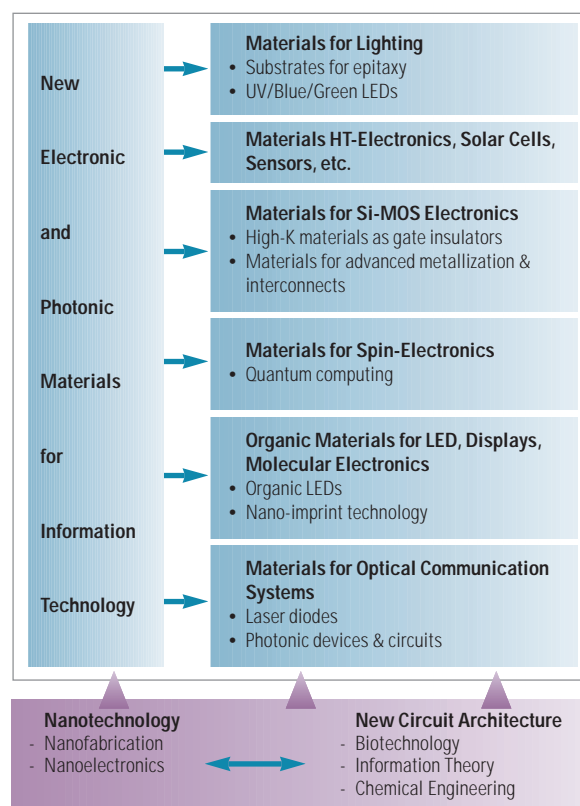
Nanomaterials is by its very nature a multidisciplinary field bringing together experimentalists, theorists and engineers, physicists, chemists and biologists. The challenges of this are accordingly big. Communication between the various disciplines can be significantly improved via coordinated research programmes, particularly by establishing a nanomaterials network or centre of excellence. Europe must meet the challenge of creating the right balance of research and training infrastructure that can be accessed by scientists from all member states if it is to remain a technologically competitive into the future.

For Europe to become competitive in the field of nanotechnology it is imperative that:

- funding for basic nanomaterials research be increased to a level comparable to that in the U.S. and Japan, and nanotechnology and interdisciplinary research be given high priority in European materials programmes.
- interdisciplinary research centres dedicated to investigating nanomaterials and the applications listed in Fig. 9.12 are established.
- industry and academia work together to develop newer, more innovative synthesis and characterization techniques.
- research into self-assembly and biomimetic materials be increased.
- computer modelling be used to predict the properties and phenomena of nano-size particles and nano-designed materials.

## 9.2.4. Electronic, Optical and Magnetic Materials

Basic science in the fields of electronic, magnetic and optical materials involves understanding and controlling electrons and electronic correlations in materials and tailored materials structures. Over the last two decades this field has uncovered many fascinating new phenomena, e.g., the quantum Hall effect (QHE), giant magnetoresistance (GMR), high-temperature superconductivity, and the fractional quantum Hall effect (FQHE). Equally breath-taking is the speed with which most of these fundamental discoveries have entered today's technology, e.g., a new high-precision standard for defining the SI unit of resistance, the ohm (using QHE), new reading heads in hard disks (based on GMR), or new superconducting devices (from YBCO materials).



**Fig. 9.13.** Research and development of new materials for the Information Technology Summary of potential research areas with inputs from Nanotechnology and integration of novel architecture design concepts.

**Electronic materials** encompass a broad range of substances from semiconductors such as doped silicon, germanium and GaAs, to electronic and ionic conductors made of metals, polymers, and ceramics. Promising areas of research include organic semiconductors, nanostructured materials, quantum dots and wires, II-VI and III-V semiconductors, and self-assembling systems.

Many breakthroughs have occurred in the use of **materials for optical applications**, especially lasers and communication devices. Novel organic materials, polymers and ceramics with tailored optical properties have all been developed. Optical materials research is one of the most innovative and rapidly developing fields of materials science and is continually resulting in new commercial products and discoveries.

A renaissance in basic research of **magnetic materials** is taking place as a result of breakthroughs in colossal magnetoresistance, magnetic multilayers, magnetic properties of thin films, magnetic coupling between layers, giant magnetoresistance and nanoparticle synthesis. This flourishing field of materials science is characterized by close collaboration between experimental and theoretical

application in the next few years, but the search for new higher temperature superconductors should also continue. In particular, further work needs to be done on

- optimizing microstructures and improving critical current densities,
- searching for new superconductors with small anisotropy and high critical temperature,
- developing and improving thin film deposition techniques,
- the detailed analysis of the materials at the micro- and nanometre scale,
- promoting exchange of scientific knowledge through creation of European networks.

A possible road map for European research in these areas is given in Fig. 9.14. In order to be able to follow this, several focused European actions are necessary:

- Establishment of interdisciplinary research centres for semiconductor technology that can compete with large research institutes in Asia and the U.S.
- Increase funding for research projects examining the fundamentals and application of single electron devices.
- Initiatives in electro-optic technology to develop next-generation computers and communications, particularly laser devices and photonics.
- Long-term projects to develop spintronics, quantum computing and other future technologies.
- Formation of Centres of Excellence in superconductivity to hasten the introduction of high temperature superconductor devices for use in industry, medicine and transport.
- Greater industry-academia collaboration on ways of improving/optimizing electronic storage media and other devices based on recent breakthroughs in magnetic materials.

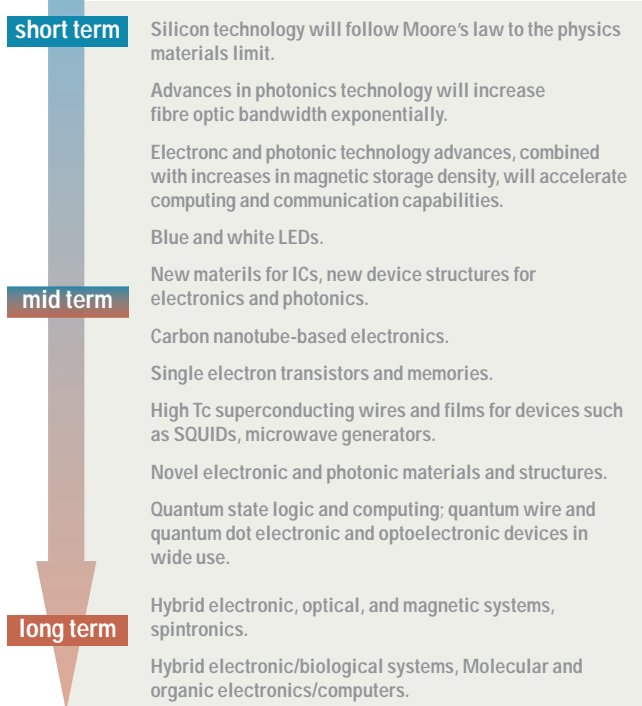


Fig. 9.14. Future progress in electronic, optical and magnetic materials in Europe

research groups. Breakthroughs are expected in the development of magnetic nanowires, perpendicular recording, magnetic non-volatile recording materials, magneto-optic layers, spin valves and molecular magnets. Most of these research activities are intimately related with nanotechnological and interdisciplinary concepts (Fig. 9.14).

Recent discoveries of **superconductivity** in MgB<sub>2</sub>, polymers and high-pressure iron show that many surprises still await researchers in this area. The ceramic high temperature superconductors will find their first commercial ap-

## 9.2.5. Materials Applications and Related Topics

Advanced materials are used in a diverse range of new and established technologies that underpin our current standard of living, and will make future technologies possible. While there is not enough room to discuss all of these here, a few examples are given of promising and topical, but also less well-known, areas of research to illustrate the diversity of needs for modern materials technology.

### (a) Materials for catalysis

In order to maintain and strengthen the world-wide leading position of European catalysis science and industry, a next generation technology platform for advanced catalysis research should be created, bearing in mind the need for full integration of homogeneous, heterogeneous and

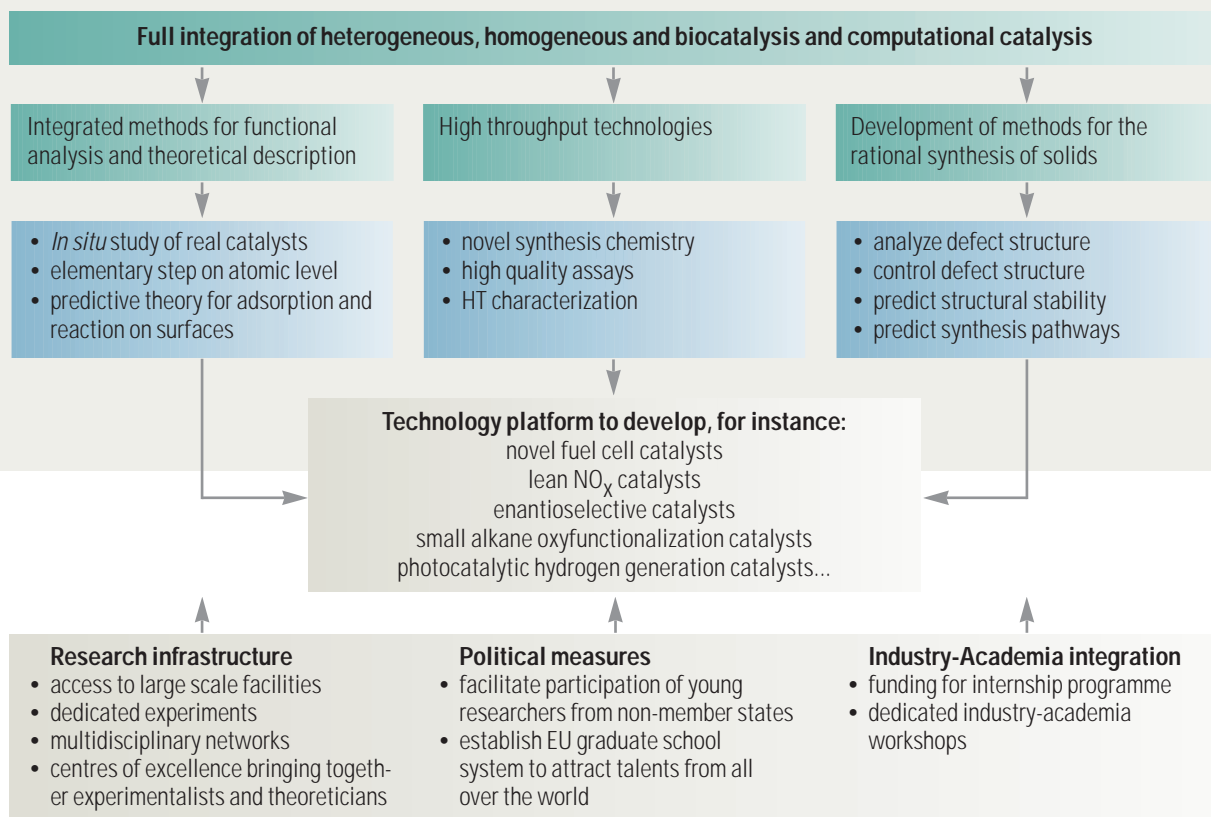


Fig. 9.15. Future research directions for catalytic materials.

biocatalysis, and including computational methods as an essential part. This technology platform should provide the enabling technology package for accelerated materials development in catalysis on the basis of an improved understanding of the controlling parameters and the processes which control these parameters on a fundamental level. The application of these enabling technologies will lead to new generations of catalysts for processes decisive for a sustainable development (Fig. 9.15). The interplay of the different factors and the role of EU actions is summarized in the following diagram.

Research topics at the forefront of catalytic science include:

- Selective oxidation
- Environmental catalysis
- Asymmetric catalysis
- Combinatorial catalysis

Recommendations for catalysis research in Europe include:

- basic research into novel materials and catalytic mechanisms at the atomic level.
- environmental legislation encouraging greater use of catalysts for pollution reduction and efficient processing.
- greater industry-academic collaboration on promising catalytic systems.

- establishment of an interdisciplinary European Catalysis Institute or Network of Excellence (see Annex 1 in Chapter 8).

#### (b) Materials for fusion reactors

Fusion technology promises to provide a limitless supply of clean and cheap electricity. Its success strongly depends on the availability of high quality structural materials that can withstand extreme environments. Over the last thirty years, however, fusion research has been conducted mostly by the engineering community, and materials improvement has been limited. Fundamental research will be vital for overcoming current materials limitations. The development of fusion materials would be expedited by greater interaction between fusion scientists and materials scientists.

#### (c) Materials for transportation

The transportation industry places extraordinary demands on the properties, performance and cost of materials because of considerations of safety, reliability, economy and design. To attain commercial success, materials engineering requires the simultaneous optimization of all these factors during the conversion of raw materials into products. The core purpose of this rigorous process of simultaneous engineering is to achieve an optimal balance between cost and product per-

formance. It is therefore recommended that Europe establish strategies for simultaneous development and engineering of materials including, among other things:

- rapid analysis techniques for complex systems
- materials with improved reliability or self-repair capabilities
- light-weight and energy-efficient materials
- smart materials for responding to vehicle conditions and providing passenger comfort.

#### (d) Materials research in space

Space platforms offer the unique opportunity to probe materials, phenomena and processes in zero-gravity environments. This space-based materials research is potentially

important for container-less studies and processes, for basic studies of diffusive crystal growth, for the growth of semiconductors with low defect densities or for the solidification of metals and glasses which may result in improved casting technologies. The apparent drawback of such experiments are the very high costs and risks involved. It is thus recommended

- to further develop a European space-based materials science programme in a thoughtful manner which includes a careful analysis of the objectives and success probability of the individual materials science projects. For microgravity studies which can be carried out within a couple of seconds it is also advisable to consider ballistic rockets and fall towers as alternatives.

## 9.3. Materials Interdisciplinarity

Materials science is by nature an interdisciplinary field, traditionally spanning engineering, chemistry and physics. The future of materials science will be in the further integration of other disciplines such as biology, medicine and computing. Knowledge from these fields will hasten the development of materials science, resulting in new technologies, innovations and applications, e.g., organic computers. At the same time, the breadth of materials science and the phenomena it encompasses can only be understood if researchers in different disciplines collaborate to generate new insights and help solve problems. To foster interdisciplinary research, institutions should adopt a flexible structure with close contact and good communications between departments and disciplines.

Some of the most promising areas of interdisciplinary research in materials science are:

- Bio-, biomimetic and self-assembly materials
- Nanomaterials
- Computer modelling (especially multi-scale modelling)
- Smart materials
- Surface and interface science

As an example, Fig. 9.15 shows how surface and interface science acts as an interdisciplinary platform. Our ability to control the structure of interfaces on the atomic level has made it possible to create many new and fascinating interfacial structures. Solid-solid interfaces in magnetic multi-layer materials result in unusual magnetic properties (e.g.,

the giant magnetoresistance effect). A current topic of great scientific interest and high application potential is the study of interfaces between ferromagnets and semiconductors, with the objective of controlling the injection of polarized electrons into semiconducting devices. Interfaces between metals or semiconductors on one side and organic materials on the other opens up completely new fields in functional coatings and organic semiconducting devices. The controlled oxidation of surfaces may produce new nanometre-sized dielectric and tunneling barriers required for future developments in the semiconductor industry.

None of these projects in surface and interface science would be possible without close collaboration between physicists, materials scientists, chemists and (more recently) biologists. It can safely be predicted that future research will reveal novel structures, phenomena and properties which do not exist naturally and which open up the possibility of completely new functionalities.

The five research areas listed above are by no means distinct, and will also bear upon one another in an interdisciplinary manner; e.g., biomaterials designed at the nano-level (i.e. bionanotechnology) could be used in the next generation of smart devices. The materials developed through interdisciplinary collaboration promise to revolutionize industrial, medical and information technologies, and thus bring enormous benefits in terms of improved standards of living. Two ways of fostering interdisciplinary

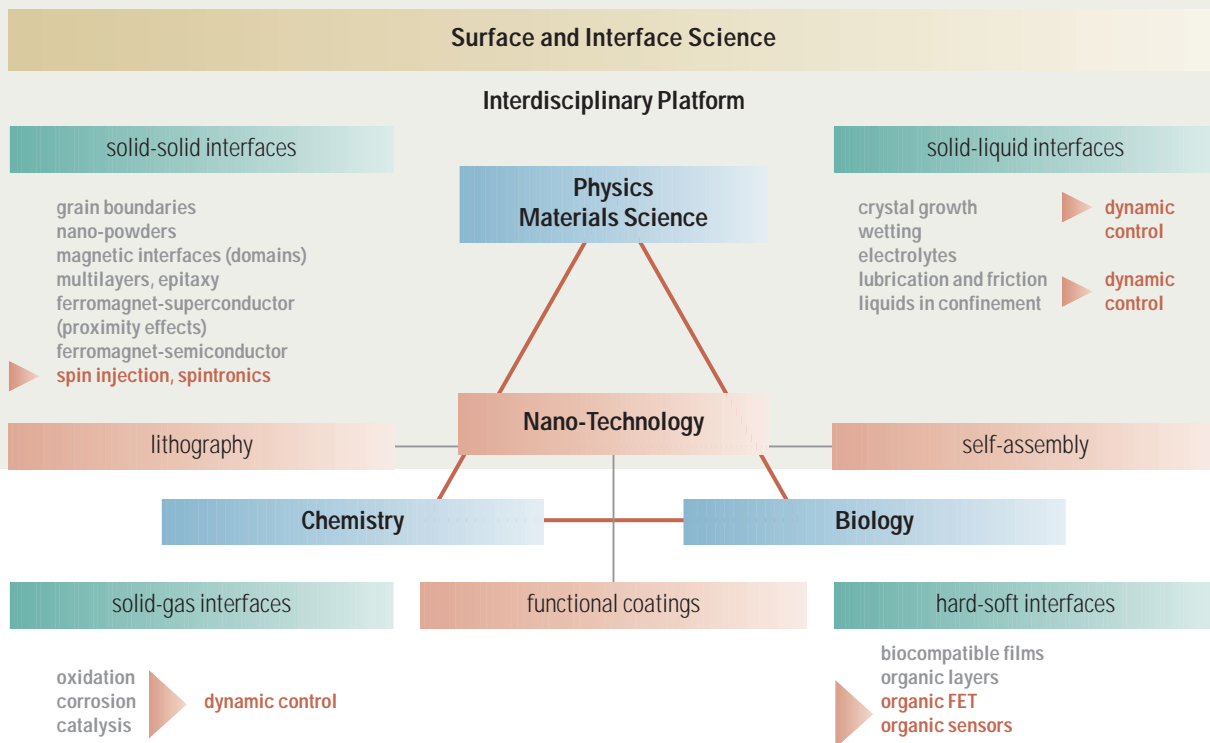


Fig. 9.15. The interdisciplinary approach to surface and interface science.

research are: i) establishing research institutes or labs in which researchers from two or more university departments or disciplines tackle related problems, and ii) linking researchers and institutes from different disciplines via networks to enhance communication and guide research in new interdisciplinary fields. Training programmes should also be highly multidisciplinary in outlook so that researchers have a flexible range of skills and can make new connections between different fields.

It is therefore imperative that:

- interdisciplinary research programmes in materials science are initiated on a European level,
- interdisciplinary European workshops, training programmes and summer schools are organized,
- interdisciplinary European research networks are set up,
- funding agencies for different branches of science coordinate their activities to make it easier for interdisciplinary projects to be established.

## 9.4. New Research Strategies and Infrastructures in Europe

### 9.4.1. Social Acceptance of Science

Steps need to be taken to reverse the trend of decreasing numbers of students in materials science courses at university, and the alienation of many members of the public from science in general. These multi-faceted issues need to be tackled from as many different angles as possible:

- restore public confidence in science by using publicly-funded science for the public good;
- improve teacher training and school curricula to make science exciting and attractive to pupils in primary and secondary education;
- engage the public on scientific issues of social relevance through TV programmes, live debates, science fairs and other events;

- improve career structures and salaries for research scientists (see below) to attract more students;
- broaden science courses to include issues of social relevance, ethics and better communication skills.

#### 9.4.2. Political Support for Science

Many areas of materials science require substantial investment and support to perform cutting-edge experiments with world-class equipment and facilities.

- European governments need to increase funding for basic science to levels similar to those in Japan and the U.S. if their economies are to remain strong in the 21<sup>st</sup> Century.
- Breakthroughs in materials science are essential for biotechnology, IT and other technologies that will determine our quality of life in the future. Materials science should therefore receive similar funding levels to these boom areas.
- Academic scientists need to be better represented at national and European levels, and should have a larger say in the science policy of the EC and Member States.

#### 9.4.3. Materials Science and Education in Europe

##### (a) Basic science education

The excitement and rewards of studying basic science need to be conveyed to youngsters as early as possible to ensure that tomorrow's Europeans value science and more of them take it up as a career. Initiatives to do this should include:

- science training and refresher courses for primary and secondary school teachers,
- visits to labs and large-scale facilities performing cutting-edge research,
- scientists visiting schools to talk to children about the adventure science, careers in science and scientific issues.

##### (b) Role of universities

Although collaboration with industry is important, the primary function of universities should be to educate students and perform innovative and horizon-broadening research. With renewed funding from their respective governments, materials science departments throughout Europe would be able to refurbish buildings and update equipment so as to attract more students and increase research output. Universities also need to be flexible enough to establish new interdisciplinary, interdepartmental centres for working on the scientific fields of tomorrow, such as biomaterials, smart materials and nanoscience.

##### (c) Human capital and research careers

Europe has enormous potential for generating innovative ideas and new technologies because of its cultural diversity and long tradition of doing top-class science. In order to realise this potential, increased mobility of researchers, particularly within the EU, is essential. Information about research opportunities in other countries should be distributed more widely, the number of international researcher fellowships increased, and restrictive immigration laws or university employment policies relaxed. Career structures and salaries for research scientists should also be improved, e.g., by encouraging universities to provide more tenured positions rather than taking on postdocs. To meet industry's demands for more materials scientists and engineers, and to reflect changes and progress within society, more women and minority group students should be encouraged to take up materials science as a career.

#### 9.4.4. Training, Mobility and Public Relations

In order to attract talented young people back to basic science and research, fundamental changes in researcher training and academic career structures are needed. European universities and research laboratories need to provide:

- more competitive salaries;
- more attractive career options for young people, including job security;
- more women students and lecturers/professors.

Greater mobility of researchers, particularly within the EC, should be encouraged to foster professional development and cross-fertilization of ideas. This would be greatly assisted by the creation of a European-wide qualification for materials scientists (EurMat) similar to that already existing for physicists (EurPhys).

As well as learning technical skills, European researchers should also receive foreign language training and communication skills. The latter is especially important if scientists are to communicate effectively with and convey their thoughts and motivations to an increasingly skeptical public. For materials science and related technologies to prosper in Europe, better promotion of this field as a discipline/career and improved public relations are vital.

#### 9.4.5. New Strategies for Basic Research in Europe

##### (a) Overall strategies

Europe should aim to be number one in as many new materials technologies as possible. It is vital that European governments and the EC coordinate research efforts via



European-wide materials science programmes and networks

- The EC should recognize the central role of materials science for technological development in its planning, funding and coordinating activities.
- The EC should set up a European Materials Council to work together with national materials societies, institutes and research councils to ensure that Europe develops first-class facilities, and to respond to the more specific needs identified in this White Book.
- Research strategies for materials science should include both small-scale and large-scale projects to take into account the needs of different Member States and research fields:

#### (b) European research networks

Creating research networks will allow a “critical mass” of researchers to be brought to bear upon complex, large-scale problems, particularly interdisciplinary areas such as nano- and biomaterials. These networks could be formalized as virtual research centres or Networks of Excellence, funded by the EC, and consisting of research groups and laboratories from throughout the EU. The growth of the Internet should also be utilized to provide high speed communications. This would allow faster flow of information, better sharing of resources, and efficient allocation of expertise for teaching and guiding and evaluating projects.

#### (c) Research facilities

Europe already has excellent experience in successfully managing and operating large-scale facilities. The number of large-scale research facilities accessible to materials scientists should be increased in the medium to long term

in order to attract the world’s best scientists and raise the standard of European research even higher. Recommendations concerning new EC-managed facilities are:

- Centres of Competence and Centres of Excellence in Materials Science and Technology should be established around Europe to house the latest apparatus and develop new analytical techniques.
- Small- and medium scale laboratories should be upgraded with modern in house instrumentation
- High Resolution Electron microscopy and High Resolution Laser and NMR spectroscopy centres need to be defined or created
- Training programmes should be offered to researchers, technicians and engineers to ensure resources are maintained and used most efficiently.
- R&D into fourth generation (LINAC-driven) synchrotron sources and pulsed neutron sources should further be pursued with the aim of constructing and running a large-scale facility over the long term.

#### (d) International collaboration

International collaboration is a vital part of modern science:

- Materials scientists should be encouraged to spend time overseas in other cultures and research environments in order to bring their newfound knowledge back to Europe.
- Nationals from regions outside of Europe should be encouraged to work in Europe through generous fellowships and research positions.
- International conferences should be held regularly and attended by researchers at all stages of their careers as they sow the seeds for new innovative ideas and fruitful research collaborations.

## 9.5. Closing Remarks

Major breakthroughs in materials science are expected over the next decade, revolutionizing the way we manage and interact with our environment. Europe must utilize its resources efficiently and maintain a critical mass of expertise to continue at the cutting-edge of research. Equally important is the promotion of materials science education and careers to the younger generation.

This White Book is intended to show the fundamental importance of basic research in materials science to modern technology, and predict the directions it will take us in the

future. As the driver behind many of today’s high-tech industries, materials science deserves the full support of research councils, governments and the general public.

It is hoped that the recommendations in this book will be implemented so that European materials science and industry prosper well into the 21<sup>st</sup> Century. It is the responsibility of educators, scientists, politicians, and other professionals to ensure that Europeans grab hold of the enormous opportunities that these developments in materials science present.