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Materials Science and Engineering Expert Committee (MatSEEC)

Materials Science and Engineering in Europe: Challenges and Opportunities

Science Position Paper

European Science Foundation (ESF)

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In the statutory review of the Expert Boards and Committees conducted in 2011, the Review Panel concluded unanimously that all Boards and Committees provide multidisciplinary scientific services in the European and in some cases global framework that are indispensable for Europe's scientific landscape, and therefore confirmed the need for their continuation.

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Cover picture:
Contact between two powder grains of a TiAl-based alloy

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Materials Science and Engineering Expert Committee (MatSEEC)

MatSEEC is an independent science-based committee of over 20 experts active in materials science and its applications, materials engineering and technologies and related fields of science and research management. Committee members are nominated by their member institutions and they maintain strong links with their nominating organisations and their respective scientific communities.

The aim of MatSEEC is to enhance the visibility and value of materials science and engineering in Europe, to help define new strategic goals, and evaluate options and perspectives covering all aspects of the field.

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Foreword

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Materials determine our environment – our world. Materials Science and Engineering (MSE), the science and engineering of making and processing materials, and tailoring their properties, are key drivers behind almost all major technological advances and breakthroughs – for example, photonic components and solid state lasers for communication technologies, Li-ion batteries for energy storage, and the performance enhancements in microelectronics, commonly characterised by 'Moore's law'. Advanced materials and advanced engineering also set the stage for the technology-based innovation of tomorrow. The societal challenges of urbanisation, resource depletion and climate change, for instance, call for a cleaner, more efficient and more sustainable economy. In turn, the efficient use of resources and energy is becoming a key challenge of the 21st century. Recent developments in materials processing demonstrate the potential that advanced processing technologies hold for the future: high performance structures and composites for products that are more energy efficient, less waste-related, better for recycling, creating more sustainable value chains. Materials Science and Engineering can provide effective solutions. Advanced Materials and Materials Engineering create new sustainable environments.

In recent years the European Commission has placed special focus on how six 'Key Enabling Technologies' (Advanced Materials, Advanced Manufacturing, Nanotechnologies, Photonics, Industrial Biotechnologies, and Micro- and Nano-electronics) can provide the instruments to accelerate the creation of innovation and the deployment of technology-based products and services, and so induced faster economic growth in Europe. Advanced Materials (and Advanced Materials Engineering) are fundamentally crosscutting and underpin the other technologies.

One of the biggest challenges in this perspective in Materials Science and Engineering (MSE) is to identify long-term trends, and to define strategic guidelines that still allow for flexibility to respond to unforeseen developments. The present report is the result of an exercise of the Materials Science and Engineering Expert Committee (MatSEEC) of the European Science Foundation highlighting selected case studies to illustrate the state-of-the-art, to identify more general technological trends and targets for the next ten to twenty years, and finally, to derive strategic recommendations for MSE programmes for implementation by the European Commission, Member States and Funding Agencies.

This report was compiled and edited by Constantin Vahlas (CNRS), the working group leader, based on contributions by members of the working group. It complements a previous joint report by the European Materials Science and Engineering Expert Committee and the European Materials Research Society (E-MRS) on 'Materials for Key Enabling Technologies'. Special thanks are due to Ana Maria Ciubotaru, MatSEEC Scientific Secretary, and the European Science Foundation for the final reviewing and publishing work.

Dr Patrick Bressler
MatSEEC Chair

Mr Martin Hynes
ESF Chief Executive

Executive Summary

Materials Science and Engineering (MSE) is a broad, diverse and multidisciplinary field. It is in continuous interaction with basic disciplines and is also contributing to meet all Grand Societal Challenges. Such a spread of MSE may well bring forth in the 21st century a new era, one of revolutionary discoveries in materials research, resulting in far-reaching changes for society. On the other hand, it requires the development of a coherent vision with subsequent coordinated actions at European, if not global scale.

Materials Science and Engineering in Europe: Challenges and Opportunities is the strategic report of the MatSEEC Working Group 'Material Challenges', based on the deliberations and contributions of its members and fuelled by discussions and working sessions involving external experts and policy makers. The aim of the report is to propose a synthetic view of selected, though representative, directions MSE should be engaged in for the next ten years. Its scope includes information about the state of the art and future challenges in MSE aimed at the public, academia and industry, and also advice to the European Commission and to the national funding agencies on their programming of MSE related activities.

The report is organised in three parts. In the first part nine significant case studies are presented, where the state of the art, barriers to overcome, process towards their solutions and scientific technological challenges to be met are organised in the form of a cumulative approach over a roughly ten-year timescale:

1. TiAl intermetallics
2. Additive manufacturing
3. Ceramic membranes
4. Powder processing
5. Smart composite materials
6. Autonomous multifunctional devices
7. Engineered organs
8. Biodegradable stents
9. Self-assembling materials

The second part presents, in an orthogonal approach, the expected impact of the case studies investigated on societal challenges, namely energy, mobility and transport; environment and climate; information and communication; and health, which simultaneously present strategic economic opportunities. The third part considers enabling points and provides recommendations on cross-cutting families of research tools and methodologies.

With the aim of maintaining academic excellence and at the same time reinforcing the capacity to innovate, national funding agencies and European institutions must consider coherent and compatible long-term strategic research plans covering the entire span from exploratory research to market implementation. This should be performed on a well-defined set of the topics presented above and especially on multifunctional and bio-based materials which are still in an early development stage and show potential for meeting numerous if not all Grand Societal Challenges. It is therefore urgently requested that these agencies and institutions focus on a mechanism allowing identification, among an almost infinity of proofs-of-concept available, of ideas which show potential to promote the state of the art towards applications. The elaboration of such a mechanism and the harmonious accomplishment of the scientific and technological progress which has been depicted through the case studies presented in this report are based on the appropriate consideration of cross-cutting families of research tools and methodologies. Last but not least, there is the need to develop cross-cutting families of research tools and methodologies. Some of them are presented below:

- To develop green chemistry and dry techniques for the processing of materials with micro- and nano-structured surfaces.
- To support materials and process characterisation techniques, both at the large instruments level and at that of R&D in the laboratory scale.
- To facilitate the invention of new analytical tools. Such tools will provide new insights to more refined material control. Progress in analytical tools is needed both in individual laboratories and in small groups as well as at large scale facilities.
- To support high throughput activities which will contribute to developing easily accessible materials and properties data banks.
- To develop multiscale modelling fed by large data banks, with the aim of (a) optimising materials processing techniques and (b) establishing the materials by design approach. MatSEEC Committee also recommends developing systematic approaches for the verification of the simulation results and the development of error estimates of the computationally predicted properties, as well as facilitation of the networking among the numerous research groups operating in this field.
- To direct funding towards strategies for more efficient use of natural resources (with the aim of improving sustainability), whether by the development of alternative materials or the improvement of recycling routes.
- To create separate evaluation panels dedicated to materials science and engineering with the aim of ensuring appropriate appreciation of the broad nature of the materials research projects, rather than having materials as a subset of physics or chemistry panels.
- To create a dedicated ERC peer review panel for Materials Science and Engineering.
- In addition to supporting pre-competitive research, European funding agencies should continue supporting exploratory research so as to maintain Europe's strength in academic research.

1.
Introduction

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Materials occupy an important place in our societies. This concerns both large distribution materials (cements, ceramics, glass, metals, polymers, etc.) and innovative devices which combine exceptional properties (nanomaterials, photonics, spintronics), advanced synthetic modes (multiscale materials) and complex combinations (composite materials). As is mentioned by Thomson Reuters, "*Fundamental discoveries in physics dominated the first half of the 20th century, whereas discoveries in molecular biology, such as the structure of DNA, dominated the second half. The 21st century may well bring forth a new era, one of revolutionary discoveries in materials research that result in far-reaching changes for society and how we live…*".[1]

Materials Science and Engineering (MSE) is a broad, diverse and multidisciplinary field. It is in continuous interaction with basic disciplines and is also contributing to meet all Grand Societal Challenges. This contribution is such that numerous reports have been produced in recent years in Europe and worldwide, with the aim of drawing a comprehensive picture and proposing coordinated actions towards the establishment of coherent strategies in the field.[2] The present report subscribes to this perspective, with a particular goal which is to contribute to the establishment of a comprehensive view of the role of MSE in the efficient development of key enabling technologies (KETs) in the EU. This is a complement to the recent E-MRS/MatSEEC document entitled *Materials for key enabling technologies,*[3] which provides a valuable basis from which to move forward, its structure being compatible with the EC's environment. However, as could be expected from the considerable extent of both the MSE and from the KET fields, the Materials for KETs document emphasises selected topics, namely materials for energy, nanotechnology and materials for micro- and nanoelectronics, and silicon photonics. Other topics such as advanced materials and biotechnology are not covered in much depth. For example, biomedical and health applications are not considered in the Materials for KETs document.

The aim and scope of this report is to propose a synthetic view of selected, though representative, directions MSE should be engaged in for the next ten years, and thus to provide the European Commission and national funding agencies with advice on their programming of MSE related activities, with the hope that such programming will be elaborated on a more coherent basis. What is aimed, *in fine*, is to contribute to the improvement of the competitiveness of Europe both in the academic and the applicative aspects of MSE and hence (a) to consolidate and to enlarge the base of scientific knowledge, and (b) to tackle the challenges European societies are facing. The type of actions to meet these requirements and the way the proposed recommendations should be implemented depends on the policy of each agency. Besides Working Group deliberations and contributions, the content of this document and the advice it contains has been

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1. Thomson Reuters (2011) *Global Research Report Materials science and technology*. http://sciencewatch.com/grr/materials-science-technology

2. See, for example, (a) Wessel, H. and Tomellini, R., eds (2012) *Technology and market perspective for future Value Added Materials*. Final Report from Oxford Research AS. European Union. ISBN 978-92-79-22003-6. (b) Adams, J. and Pendlebury, D. (2011) Evidence, In: *Global research report, Materials science and technology*. Thomson Reuters. ISBN 1-904431-29-1. (c) de Baas, A. (2010) *Research Road Mapping in Materials*, European Union. ISBN 978-92-79-14485-1. (d) Kiparissides, C., ed. (2009) *NMP expert advisory group position paper on future RTD activities of NMP for the period 2010 – 2015*. European Communities. ISBN 978-92-79-14065-5.

3. Richter, H., ed. (2011) *Materials for key enabling technologies*. E-MRS, MatSEEC, European Science Foundation, Strasbourg. ISBN: 978-2-918428-43-5.

fuelled by discussions and working sessions involving external experts and policy makers. The interactions were mainly structured around two workshops organised by MatSEEC, the first in Leuven in March 2012 and the second one in Darmstadt in September 2012.

The first workshop, gathering 16 experts from various material sciences disciplines, considered the profiling of 11 classes of materials:

1. Multi-functional materials
2. Multistructural materials
3. Metamaterials and artificially structured functional materials
4. Nano-enabled materials in metallurgy, forestry, energy efficiency, etc.
5. Bio and bio-based materials
6. Bio-inspired materials
7. Materials for targeted surface properties
8. Metals
9. Ceramics, including cement and glass, and composites including natural fibres reinforcement
10. Polymers
11. Soft materials

This preliminary step to the present synthesis allowed an overview to be made and these different classes of material to be characterised, taking into account: their state of maturity, relevant research tools and concepts as well as their environmental impact, potential application and markets.

The conclusion of this workshop led to integrating the 11 classes into three overarching clusters, namely advanced classics, bio- and functional materials, and nano-materials. For each of these clusters, priority topics and perspectives in the short, medium and long term were discussed and identified.

The second workshop gathered 20 experts and representatives from European research organisations, and aimed to consider the outcomes and findings of the Leuven discussion, trying to synthesise them and position them in the wider European material science policy arena. In this context, the main conclusions can be summarised as follows:

1. It appears obvious that the various fields of material sciences are increasingly connected to other fields of research and technology development. The case of biomaterials, the general environmental impact of materials and their processing are striking illustrations of this point. This increasing interdisciplinarity impacts on the way scientific programmes are managed, e.g., how to control the quality of the evaluation of proposals and how to involve different communities. Furthermore, the impact of this connectivity on the education curricula also needs to be established.
2. The lack of public funding for pre-competitive research leads groups to enter into collaboration with (a single) industrial partner at a very early stage. Considering IPR issues, this was perceived as a major constraint in setting up open collaboration, maturing the knowledge and making new techniques and products available.
3. The issue of standardisation of techniques was identified as a requirement to improve the research output. An example here is the need to standardise optical and contact methods (such as scatterometry) in the semiconductor industry to measure grating periods and structured surfaces. These methods present issues that still need to be addressed. They include, but are not limited to, the effect of imperfections, how to measure increasingly smaller areas and computing time. Another, prominent example of lack of standardisation that complicates the data analysis in biomaterials science is the wide variety of assays that have been used to report the efficiency of different devices for the optimal peripheral nerve regeneration.[4]

In addition, the following cross-cutting topics were confirmed as being of critical importance to improve the research process across the material sciences' board:

- Analytical tools and characterisation methods
- Combinatorial materials science
- Data storage and processing tools
- Simulation
- Surface science as an enabling technology
- Multifunctionality
- Availability of natural resources
- Recycling

The MatSEEC Working Group 'Material Challenges' based their deliberations on the outcomes and findings of these two scoping and structuring events and produced the present report.

The strategic report is organised in three parts. First, it presents nine significant case studies in the field of metals, ceramics, multifunctional materials, bio-, bio-based and bio-inspired materials.[5] Second, it discusses, in an orthogonal approach, the expected impact of the case studies investigated on societal challenges: energy, mobility and transport; environment and climate; information and communication; and health. Finally, it considers enabling points and provides recommendations on cross-cutting families of research tools and methodologies.

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[4] Yannas, I.V., Zhang, M. and Spilker, M.H. (2007) *J. Biomaterials Sci.*, Polymer Ed., 18:8, 943-966.

[5] Note that we deliberately avoid the topics that were covered in detail in the Materials for KETs document.

2.
Case Studies

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The presentation of the case studies is organised in the form of a cumulative approach over a roughly ten-year timescale, rather than as a linear process. The aim here is not to develop roadmaps; this is an industry-driven task for a particular technological area (e.g., microelectronics) which is incompatible with the position of MSE at the crossroads between scientific disciplines and societal challenges. It is rather aimed at allowing case-based reasoning, depicting the current state of the art, the barriers to be overcome, the process towards their solutions (including the milestones), and the scientific and technological challenges to be met. It is thus expected that information will be available to feed a 'retrieve, reuse, revise, retain' process to approach other materials cases. In addition, these studies should provide illustration of cross-cutting families of research tools and methodologies, and of general concerns in the area of MSE.

The selected case studies are sequences of achievements of particular targets, either autonomous or intermediate, in the course of attaining more integrated/global targets and of creating new solutions. Although such a sequence in each case study clearly illustrates the forthcoming evolution (in the form of an initial and a final state), it does not account for the kinetics which will control the transition from one state to the other. The pace with which such evolutions will occur depends on progress in transversal factors, including education and training, tools, facilities and infrastructures, computational techniques, methods and design, funding and outreach. These factors have variable impacts on the barrier between two sequential states; they are separately analysed in MatSEEC.

It is worth noting that the case studies investigated concern domains where either Europe has strengths, and/or where there is a potential and a need for industrial production to take place in Europe. The first four case studies (TiAl intermetallics, additive manufacturing, ceramic membranes, powder processing) deal with metallic and ceramic materials. Europe traditionally plays a leading role in these fields. They are vital for the future of the continent because of their impact on energy, environment, health and production (cost, flexibility, raw materials availability) issues. However, without adequate support Europe's advance will be quickly lost. Research funding policy should include sustainable support of basic research together with applied research driven by industrial needs and with visionary/strategic research on topics such as life-cycle analysis, recyclability and availability of raw materials.

The remaining five case studies concern smart composite materials, autonomous multi-functional devices, engineered organs, biodegradable stents and self-assembling materials. These categories are still in an early development stage. Their potential is widely recognised as the next generation materials in terms of advanced functionality and sustainability, although important basic concepts are still lacking such as: how to achieve bio-inspired materials that can replace, for example, our civil construction materials or our petrochemically-sourced polymers? How to design reconfigurable, autonomous, self-sensing materials? What would be an engineering approach to complex self-assembled materials? How to engineer new organs for humans and new bio-inspired platforms for bottom-up materials synthesis? There is currently very active research worldwide in multifunctional and bio-inspired/bio-based materials and devices. This research is very fragmented in Europe. The case studies chosen

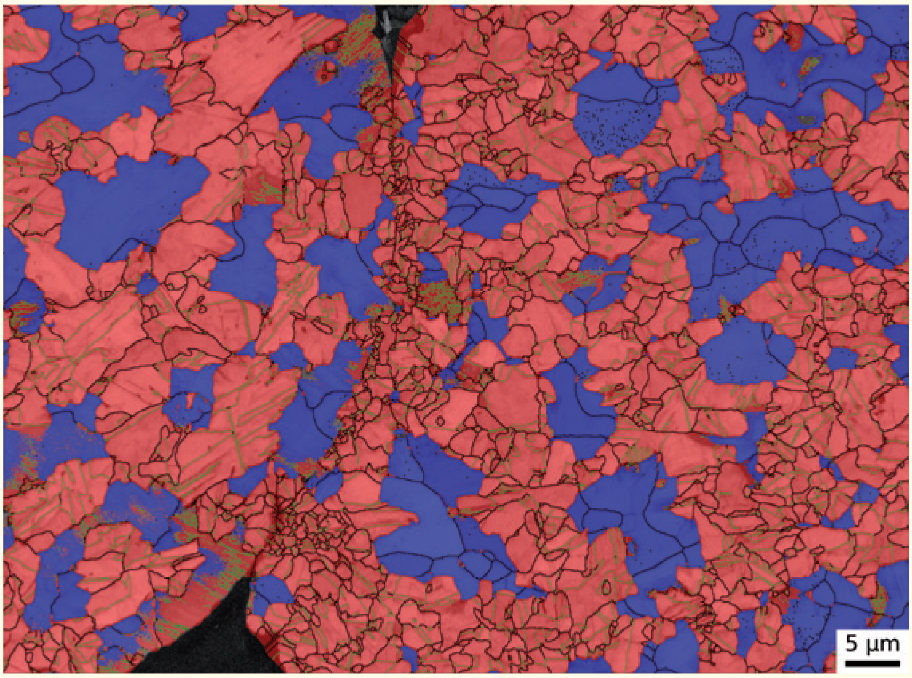

Figure 1. Contact between two powder grains of a TiAl-based alloy at the early stage of spark plasma sintering (SPS). EBSD analysis allows detecting α and γ phases (blue and red, respectively) as well as grain and twin boundaries (black and green, respectively). SPS induces $\alpha \rightarrow \gamma$ phase transformation and dynamic recrystallisation.

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highlight the importance of cross-cutting families of research tools for the development of these materials.

2.1 **TiAl Intermetallics**

The state of the art in metallic systems for turbine blades, aero engines and gas turbines is the use of Ni superalloys. The implementation of TiAl intermetallics in applications involving moderate temperatures is foreseen within the objective to decrease the weight by up to 50% (Figure 1). The challenges here are to increase the ductility of TiAl intermetallics at room temperature, to improve the creep properties at temperatures up to 700 °C, and to develop alloying through optimised heat treatments. Such an improvement requires insight into the fundamental properties of these materials on all length scales. In a longer time perspective, the challenge is to develop processing routes which integrate recycling and reuse. At that point, another challenge will be the determination and control (also involving non-destructive testing) of degradation and of failure mechanisms of such alloys, including corrosion (chemical, galvanic), mechanical, thermal, bio-fouling, irradiation, wear and especially combinations thereof. Processing of TiAl intermetallics is currently based on casting technologies, for which Europe has a leadership that should be retained for future developments. In the longer term, challenges are the use of TiAl intermetallics in hybrid and/or composite materials, safety and quality issues, and multiscale-multiphysics modelling.

2.2 **Additive Manufacturing**

Additive manufacturing (including popularly known ‘3D printing technique’) is presented here as a paradigm of advanced processing technologies. Europe is currently leading in this field and it is strategic to maintain and to increase this leadership since there is only limited research in this field in other regions in the world. Further development of additive manufacturing technologies will be possible through progress in standardisation and in non-destructive testing, allowing for improvement of the quality of the fabricated pieces. Once such progress is achieved, a next challenge will be generalisation of metal additive manufacturing. In parallel, the quality of raw material (feedstock) must be improved. This will in turn allow the production of more homogeneous parts with less gas trapping, limited porosity or oxidation and with reduced cost. Replacement of powders by wires and mass reduction through topological optimisation and

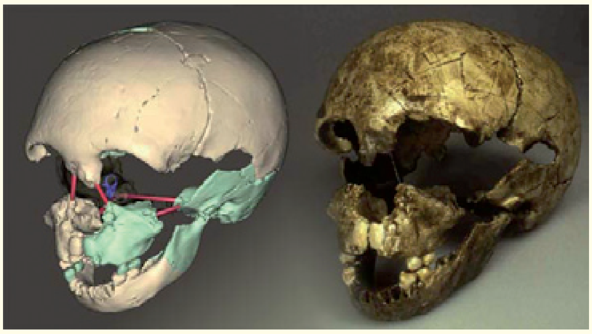

Figure 2. Virtual and stereolithographic reconstructions of the Devil’s Tower Neanderthal child.

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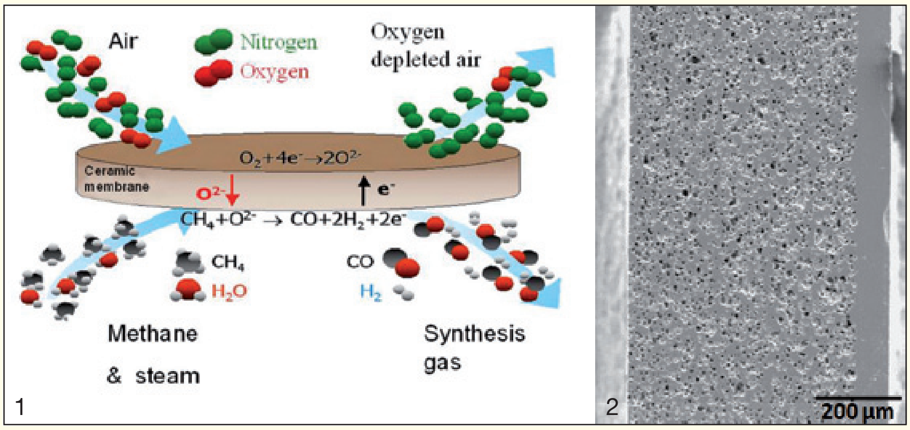

Figure 3. (1) Short description of the ceramic membrane for the separation of oxygen from air for the production of hydrogen through the partial oxidation of methane (POM) or oxy-combustion at high temperatures and (2) Bilayer membrane with porous support and dense perovskite layer for oxygen separation.
© T. Chartier and P-M. Geffroy (SPCTS) and P. Del Galo and N. Richet (Air Liquide)

functionalisation are longer term challenges. *In situ* process monitoring and, as for TiAl intermetallics, insight and control of degradation mechanisms through non-destructive testing are challenges to be met in order to make progress towards the processing of large (larger than 1 m) parts for technological applications. In this way, it will be possible to fabricate parts for application domains such as medicine, aerospace, energy (including nuclear fusion) and security (Figure 2).

2.3 **Ceramic Membranes**

Due to their chemical and thermal stability, narrow pore size distribution, high porosity, high flux, mechanical strength (enabling back flushing), microbiological resistance and long lifetime, ceramic membranes are foreseen for filtration purposes in a broad range of industries such as biotechnology and pharmaceutical, dairy, food and beverage, as well as chemical and petrochemical, microelectronics, metal finishing and power generation (Figure 3). Current barriers to their efficient implementation in such fields are scaling up and enhanced interaction (information exchange) with industry. Mid-term challenges are more efficient (generalised) access to large instruments for improved processing of these materials and for better understanding of their properties, more generally through extended use of analytical tools. This should allow new design of membranes, particularly targeting increased efficiency and at the same time improved recycling. Further progress in this field concerns multiscale modelling and simulation with subsequent understanding of transport mechanisms and materials properties. This in turn should contribute towards improved transport properties at low temperature and should confer ceramic membranes with targeted functionalities through optimised formulation design and structure and through the application of coatings on their surface, with complementary functionalities. The next challenge is integration of ceramic membranes. At that point, a barrier could be funding of demonstrators at pilot scale. Longer-term challenges are tooling for the fabrication of large parts. Meeting these challenges should allow processing more reliable parts through robust processes with less waste and implementing ceramic membranes in various technological applications including new generations of fuel cells or chemical reactors.

2.4 **Powder Processing**

The present challenges in powder processing routes, both colloidal and in suspension, are the control of the 3D-structure rheology through the *in situ*

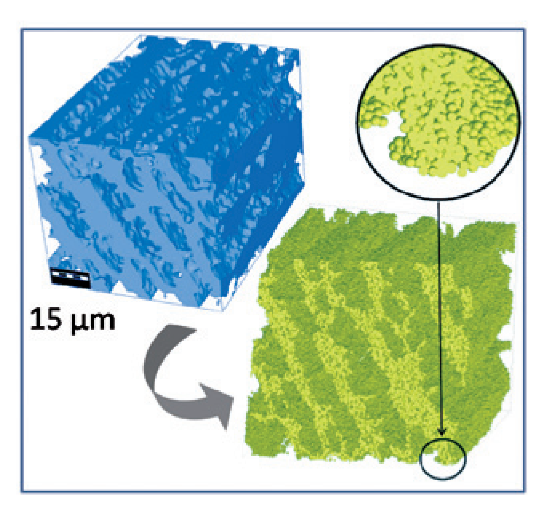

Figure 4. Processing, characterisation, simulation and design of multiscale microstructure: Anisotropic composite ceramic electrodes consisting of large (~ 15 µm) and small (~ 300 nm) pores made by directional freeze casting, characterised by 3D X-ray nanotomography (ESRF). Numerical model from image processing for the computation of effective properties (conduction, fracture, gas transport, etc.), illustrating the coupling of tomography and simulations.
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coupling of new analytical methods. The baseline here is to implement existing technologies in such complex systems. Once these challenges are met, it would then be possible to tackle two additional ones, namely the simulation of the hydrodynamic behaviour of such systems and their use in additive manufacturing. In the medium term, it will be necessary to experimentally investigate and to control the reversible interaction potential among particles so as to consider smart particles in powder processing. This term includes particles with tailored shape, size and surface chemistry. Use of such smart particles raises the challenge of their characterisation, especially for those whose size does not exceed 5 nm, for which toxicology and carcinogenesis studies will continue. Integration of particles with tailored properties in powder processing should be considered both in top-down and in bottom-up approaches. Longer-term challenges in this case deal with reverse modelling and with mass production (Figure 4). Meeting these challenges should allow the nanostructure of metals and ceramics to be assessed, controlled and tailored.

2.5 **Smart Composite Materials**

Smart composites combine a range of functionalities to produce a material that has better performance than its individual components. Traditional metal or ceramic-based composites are well known and, for example, the multiferroic effect, where the electric properties of the material can be manipulated by an external magnetic field and vice versa, can be obtained through the formation of multilayers of piezoelectric and magnetostrictive materials. A first challenge in this field is the fabrication of organic-inorganic (for example, polymer-ceramic) smart hybrids, such as the bone. Multiscale modelling is a first milestone in this case. A short- to medium-term barrier is the limited processing compatibility with current technology. Interesting functional organic materials to integrate into smart composites are, for example, molecular or polymer semiconductors, where applications such as organic light emitting devices (OLED) and solar cells are reaching the market place (Figure 5). Advantages of the organics include low cost, mechanical and chemical flexibility, and ease of processing. As charge transport is hindered at grain boundaries, the molecular thin films are either grown as amorphous layers or as single crystals, but the latter are much more difficult to process. A particularly exciting development for miniaturisation and increased efficiency is the advent of molecular nanowires, which can be grown from solution or from the vapour phase.

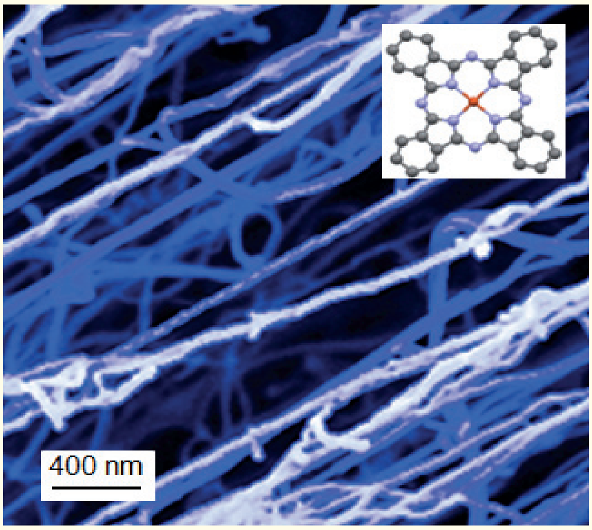

Figure 5. Crystalline nanowire of the molecular semiconductor copper phthalocyanine (see molecular structure in the inset) with diameters down to 10 nm, aspect ratios close to those of carbon nanotubes and deposited at room temperature over large areas.
© H. Wang *et al.* (2010) ACS Nano 4: 3921

The integration into more complex multifunctional structures, where, for example, a magnetic field is used to modulate the efficiency of an OLED, or where the organic layer is used as a spacer between inorganic-ferromagnetic leads in spin-valve configurations, are currently actively explored in the recent field of molecular spintronics. Mid-term milestones at this stage are combination of sensor and actuator function in one composite, the capacity to access a large number of responsive materials for targeted applications, and the recycling or the recovery of valuable materials. Longer- term barriers are, at the fundamental level, the need to access and to control the correlation between properties and structure and, at a technological level, the implementation of smart composite materials into chip for effective utilisation. A milestone at the same time scale would be to extend the types of functionalities within one composite.

2.6 **Autonomous Multifunctional Devices**

Autonomous devices (including combined sensor-actuator systems) are defined as having energy harvesting circuitry, on-board electronic circuitry, and signal transmitter circuitry (e.g., RF) using a transmitting profile that includes a plurality of pulses (Figure 6). Autonomous devices are often limited to one single function. However, considering the high potential for their implementation in different applications, there is actually intense

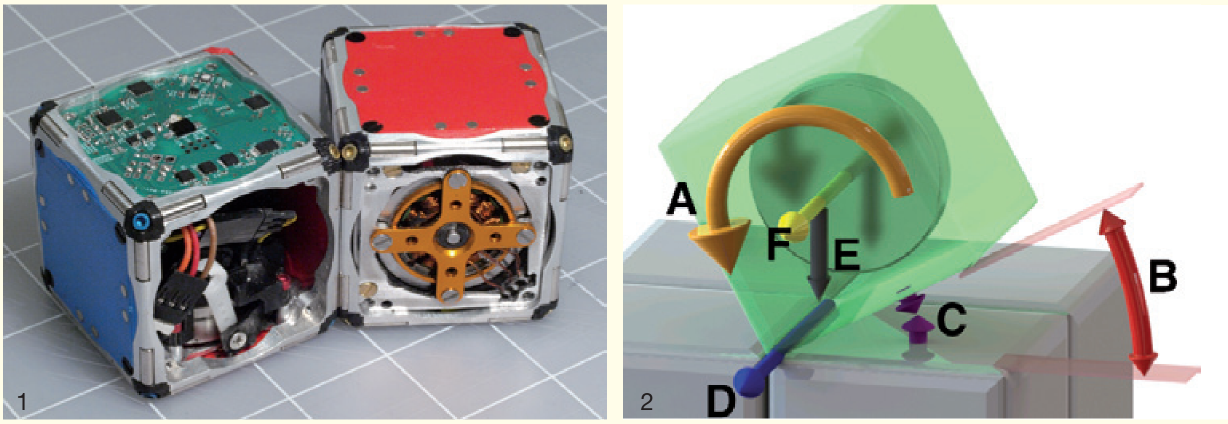

Figure 6. (1) M-Blocks, 50 mm self-assembling and self-reconfiguring cubic robot using pivoting motions to change its intended geometry; (2) When a torque (A) about an axis (F) causes the module to pivot through an angle θ (B) about an axis (D), the modules experience additional forces: downward force due to gravity (E) and magnetic force from the face-to-face bonds and any edge bonds being broken (C).
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academic research to multiply their functionalities. Current barriers are limited signal transfer (antenna size), still too high power and energy consumption, integration of energy harvesting and/or storage, and limited reliability of Pb-based materials. The background activity is miniaturisation and short-term milestones are replacement of Pb in piezoelectric materials, compatibility of fabrication with small scale technology, reduced degradation combined with increased reliability, and improved engineering to meet a combination of functions. Mid-term challenges are the fabrication of bioactive composite scaffolds which are multifunctional and more general biocompatibility in terms of fate of nanoparticles and ion release. A barrier to meeting these challenges is integration in terms of materials compatibility, the level of which depends on the device and its complexity. Milestones are sensors for early warning, multiscale materials simulation, autonomous response with actuators and availability of sensitive innervation in medical implants. Long-term challenges are integrated devices based on multifunctional materials and corresponding barriers are clinical trials and regulation and product (market) approval for medical use.

2.7 **Engineered Organs**

The context in engineered organs is an ageing population, increased obesity and poor physical activity (Figure 7). These elements together impact bone disorder together with complementary conditions such as osteoporosis and bone fractures. Tissue scaffolds and controlled release delivery devices represent the actual state of the art in this case study. Further progress here requires 'biologisation' of the biomaterials, i.e., a stronger biology insight in MSE. Also, or as a consequence of this requirement, there is a need for a more multidisciplinary approach to the field, through the collaboration in R&D among biomedical experts, cell biologists and material scientists. A first sequence of milestones in this field are improved and optimised biomaterials with targeted mechanical properties, new biomaterials for regenerative medicine, a selection of optimised biodegradable biomaterials for tissue scaffolds, and biomaterials for regenerative medicine based on bio-processing methods. These milestones lead to the challenge of vascularisation of scaffolds, with three subsequent milestones: improved bio-reactor technology; design and reliable fabrication of 3D scaffolds which are bio-resorbable with time and load-bearing conditions; and solving of ethical aspects. Long-term challenges are angiogenesis and reproducible and low-risk bone regeneration, and also injectable cell scaffolds. Foreseen barriers at this point are the production of organs derived from patient's own cells, cell printing and tissue engineering. A significant milestone is the up-scaling for industrial production with corresponding barriers: clinical trials, regulation and product (market) approval.

2.8 **Biodegradable Stents**

The principal motivations for R&D in biodegradable stents are children's diseases and the need for short-term treatments, e.g., aneurisms. Current research focuses on tailoring chemistry and topography. Short-term barriers are cell banks and stem cells, i.e., the availability of relevant cells, and understanding of the impact of degradation products and of degradation process on the control of the degradation rate. Milestones are the development of appropriate

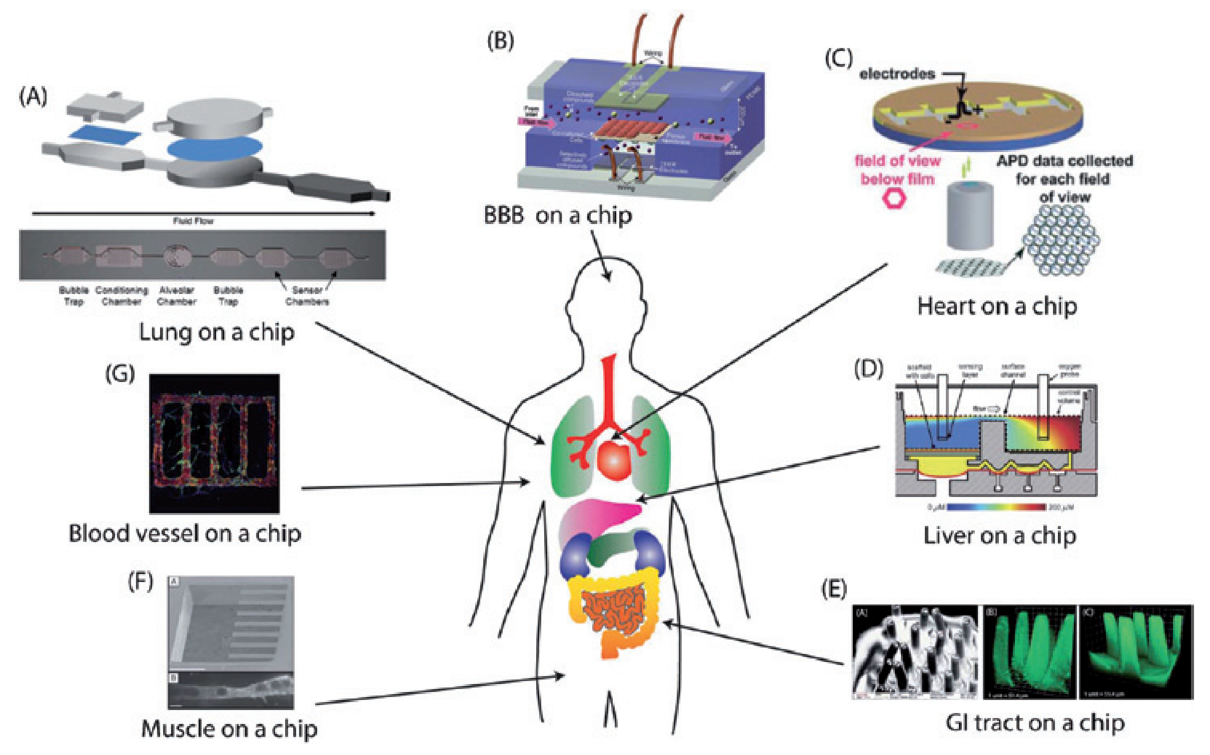

Figure 7. Microfabricated organ systems mimicking various organ tissues. (A) Lung on a chip device modelling an alveolus and layout of fluid side of lung-based body-ona-chip device fabricated in silicon. (B) BBB on a chip, consisting of two perpendicular channels separated by a membrane. (C) The contractility of heart tissue is measured using the muscular thin film (MTF). (D) A microfluidic bioreactor for 3D liver tissue engineering. (E) Microscale hydrogel scaffold mimicking the intestinal villi geometry. (F) Cantilever for detecting myotube contraction. Above: SEM micrograph of silicon cantilever array. Below: Confocal micrograph detailing top down view of a single cultured myotube on a cantilever. (G) Microvascular network in 3D tissue scaffold made of collagen matrix.

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design, surface functionalisation and improvement of the mechanical properties, namely the stability of the stent (Figure 8). At that point, motivation for further research would be the decrease of thrombosis risk, and the use of non-metallic stents so as to avoid artefacts in magnetic resonance images. Mid-term challenges are Mg-based alloys or biodegradable polymers and the controlled release of various drugs, e.g., from multi-layered structures. Manufacturing techniques and corresponding processes are required to meet these challenges and this is a mid- to long-term milestone, together with stent miniaturisation for brain applications. A corresponding challenge at this point is the ability to produce biodegradable stents with predictable behaviour, namely degradation rate. As is the case for previous case studies on biomaterials, long-term barriers are clinical trials, regulation and product (market) approval.

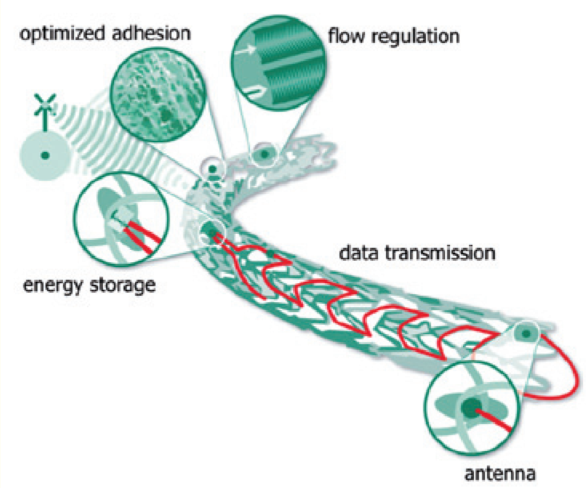

Figure 8. Scheme of an intelligent stent showing surface modification for optimised adhesion, flow regulation by bio-inspired micro- and nanostructures, as well as an antenna for data and energy transmission, which is needed for the operation of integrated sensors and actuators.

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Figure 9. Demonstration of self-assembly and molecular chirality, or right-handed and left-handed patterns of attraction. Opposing attraction patterns in the self-assembly units allowed for the parts to sort themselves when combined and shaken randomly. The yellow units and black units eventually self-assemble into two distinct structures, demonstrating error-correction throughout the assembly process. The molecular structures in this exhibit were based on the Polio Virus capsid.

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2.9 **Self-Assembling Materials**

There is fairly good knowledge of biological systems which is translated into the ability to fabricate simple objects with self-assembly processes. The first milestones towards more complex structures are the modelling of assembled objects and the development of concepts for assembly from individual building blocks (Figure 9). These should be made at the nanoscale as the starting point. Progress in self-assembling materials is subject to three conditions: cost reduction; development of dedicated instruments on atomic level; and the biological production of the building blocks for self-assembly. Mid-term milestones deal with 3D structures, whose assembly are protein-directed or are obtained from self-folding polymers. Once such structures are assembled, a barrier would be their integration into devices, with a subsequent challenge on the modelling and the simulation of assembly processes. Self-assembly in different scales is a long-term milestone, with challenges here to engineer stable, macroscopic structures and, ultimately, to assembly complicated objects.

3.
Applications

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The barriers, challenges and milestones for the nine case studies on MSE presented in the previous section are reorganised in the present section *vis-à-vis* five societal challenges which simultaneously present strategic economic opportunities: energy, transport, climate, information and communication, and health. While in the previous section emphasis was put on the – mainly – technological and scientific progress-based evolution in each case, the objective in this section is to position the materials and challenges as a facilitator to cross the sequential steps in each challenge.

3.1 **Energy**

It is recalled here that the energy challenge is covered in detail in the Materials for KET report and the main conclusions and recommendations of the present document are similar: the need for higher efficiency and lower operating temperature for fuel cells, for appropriate fabrication process of polymer membranes, for novel, low-cost catalysts operating at reduced temperature in, e.g., microstructured reactors, for portable miniaturised energy harvesting devices, and for energy storage. Identified short-term barriers are the upscaling to real system size and the reduced lifetime of ceramics for Solid Oxide Fuel Cells (SOFC). Foreseen mid-term milestones are materials for smart grids and nuclear fusion, compound semiconductor nanoparticles for solar energy applications (thin film photovoltaics and water splitting), ultra-high strength wires for ultra-strong electromagnets, wings for wind turbines (piezomaterials, carbon fibre reinforced composites), ceramic-materials-based highly reliable components for rotating parts in gas turbines, magnetocaloric refrigeration, solid-state caloric effect ferroic materials. On a more visionary scale, high efficiency low cost thin film solar cells at fully competitive cost and lifetime, low power technology such as lighting solutions using organic and inorganic LEDs and spintronics, green catalysts, artificial leafs and multimaterials for ultra-high divertor parts for nuclear fusion should also be developed.

3.2 **Transport**

In general terms, the energy dissipation needed for transportation purposes can be reduced by the further development of affordable high-strength materials, including steel, a material for which Europe still keeps up with its Far East competitors. However, without sufficient effort, the risk is real that it would be left behind in the near future. The state of the art in the aeronautics sector refers to Al alloys, for which the short-term expectation is higher strength and easier joining. Milestones concern non-destructive techniques, and insight in ageing through reliable accelerated testing and determination of remaining potential. These milestones are of major importance for the implementation of polymer matrix composites in this sector. Two additional short-term milestones which also refer to the energy challenge are low cost, widely available thermoelectric generators, and hydrogen storage in transport applications and especially metal hydrides which are safe, accessible and present high output. There is a strong need for surface treatments in this sector and for this reason a mid-term milestone is the development of combinatorial processing of multifunctional (including protective) coatings. Such coatings should also contain new materials families such as complex intermetallic alloys. Concerning bulk materials, mid-term milestones are high strength metals which are also ductile and further implementation of TiAl alloys in aeroturbines, namely in vanes and blades. At this point, a barrier in processing science is the development of hot isostatic pressing for large scale metal or ceramic structures. Longer-term challenges are materials for Li-ion batteries and vehicle and automotive engine parts from metal matrix (nano) composites. Longer-term milestones are Mg lightweight alloys in aeronautics and new, shape memory alloys for actuators, while in a more visionary perspective additively-made single-piece space satellites (through alloy specific design) are foreseen.

3.3 Climate

Short-term milestones in the environment and climate societal challenge concern building materials, namely those which are energy efficient (e.g., dye-sensitised polymer solar cells) and those obtained through recycling (e.g., ashes and again polymers). In parallel, there are needs for membranes for clean environment and polymers, ceramics and/or carbon-based materials for CO_2 removal. Materials for sensors are another group of interest in the short term, with particular requirements for multifunctionality in the context of environmental monitoring. Underlying requirements for all these materials families are *ad hoc* processing science. Reliable and inexpensive water treatment and storage is a mid-term challenge together with autonomous water treatment units for remote locations. In a longer perspective, bio-based and self-assembled new materials will present potential interest to face needs in the environment and climate challenges.

3.4 Information and Communication

New (ceramic) materials for lasers, including high power ones, new optical fibers, and polymer composite (light) materials for telecommunications satellites are short-term milestones in the information and communication domain. There are significant, short-term needs for inexpensive electronics such as plastic ones for smart labels or low cost printed ones made from organic conductors and semiconductors with corresponding milestones concerning the production of throw away and flexible devices with acceptable lifetimes. In the field of MEMS, the needs are for bulk-metallic glass composites while in the sensors family, the short-term challenges concern multifunctional coatings and integration in structural materials. In a mid-term perspective, needs are expressed for high definition, low power screens for portable electronics, for low power, high speed field effect transistors made from assemblies of nanotubes into arrays, and especially for integrated optical switch on waveguide quantum dot resonators. Long-term milestones in this area are the development of large scale processes for nanotube FET in industry, of tunable RF devices and swarms or networks of sensors as well as autonomous actuators. Also, graphene-based transistors and autonomous devices, either multifunctional or for sensing and actuation and new quantum-base technologies are extremely promising. In both cases small, possibly micro-, even nanometric size will be required.

3.5 Health

Ageing and sedentarisation of the population are the driving forces for research in materials for health. Short-term milestones in this area are autonomous bio-sensors, non-invasive therapy and drug delivery, and polymeric coatings, biomedical and also architectured, for digital lenses. Additional needs concern simple biodegradable implants, scaffolds with angiogenic potential and sensors. For the latter, advanced polymers and other organic materials are needed for mobile patient monitoring. Mid-term milestones are lab-on-chip for fast, portable, multiplex diagnostics, implants with added biological factors, bioactive glasses with therapeutic ion release ability, with additional pronounced needs on surface chemistry functionalisation for cell expression. Longer-term milestones are artificial muscles, superconductors and materials for nano-bio medicine, namely magnetic nanoparticles for cancer treatment. Also, dual-function (theranostic) optical fibres, resorbable bio-compatible Mg-based devices (for stents and orthopedic applications), patches for cardiac regeneration, biodegradable stents, artificial cellular factories for drugs, materials with tunable stiffness for implants and lab-on-chip for module organs (all/tissue dips). Milestones in a more visionary perspective are nanoparticles for combating infections and cell printing scaffolds.

4.

Enabling Points and Recommendations

Europe must consider a long-term strategic research plan covering the entire span from exploratory research to market implementation on a well-defined set of the above presented topics and especially on multifunctional and bio-based materials which are still in an early development stage. It is therefore urgently requested that the European Commission focus on a mechanism allowing identification, among an almost infinity of proofs-of-concept available, of ideas which show potential to promote the state of the art towards applications. The elaboration of such a mechanism and the harmonious accomplishment of the scientific and technological progress, which has been depicted through the case studies presented previously, are based on the appropriate consideration of cross-cutting families of research tools and methodologies. Last but not least, there is the need to develop cross-cutting families of research tools and methodologies. Some of them are presented below.

4.1 **Synthesis, Processing, Production, Nanotechnology**

Materials preparation includes soft chemistry synthesis, materials shaping (including the already classical nanomaterials such as particles, tubes, layers) and alloy processing. It also includes the replication of artificially created nanostructures, either by optical lithography for the large volume production of electronic devices, or the direct write lithography, such as electron beam lithography, which is slow and costly. A wide range of synthesis tools and routes are applied depending on material system and configuration. In particular, dry deposition techniques, such as physical vapour, chemical vapour and atomic layer deposition, show promise to create architectured multifunctional nanostructures in the form of films and coatings. Europe has a very strong scientific position in this field, including nanotechnology.

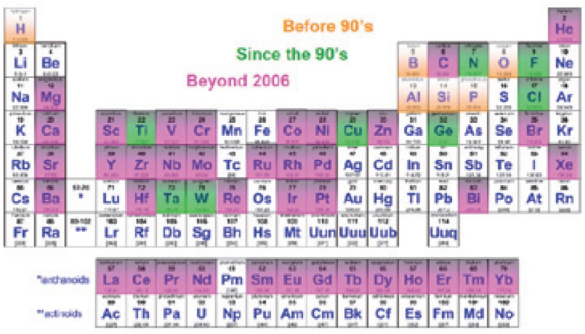

Figure 10. Elements employed in Si technology. Up to 1990, the fabrication of Si-based electronics involved merely 6 elements, namely Si as the fundamental semiconductor material, B and P for doping, O for making insulating layers, H for passivation, and Al for the interconnects. In the next decade the basic six elements were complemented by Ti, Ta, W, Cu, Ge N, F, and Cl. Today, approximately 50 elements, in particular also rare earth elements, are used in the manufacturing process.

The latter has a strong materials science component (Figure 10) and for this reason progress in materials science (e.g., mastering the art of making the structures, functionalising the surfaces, and assembling the nano-devices in a functional device) is at least as important for driving innovation as the capability of making things smaller. In this perspective, surface nanostructuring beyond thin film technology, i.e., combining nanostructuring in more than one dimension, is an important challenge to be met in the next decade. Such nanostructuring can be obtained considering various technologies, such as optical lithography combined with self-assembling, e-beam lithography and local probe lithography (Figure 11). Controlled design of surface roughness

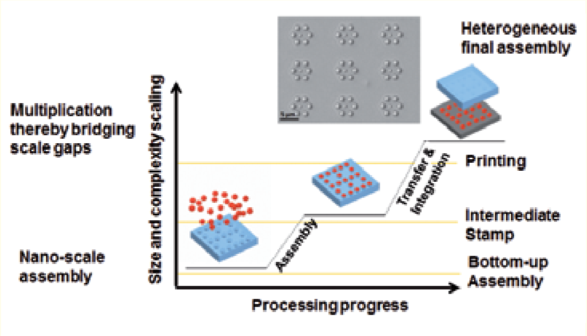

Figure 11. Generic principle of bottom-up assembly for scalable production of complex structures: (1) Parallel assembly of functional units exploiting unique characteristics of nanoscale materials properties. (2) Multiplication of the initial fabrication process using for example printing techniques. (3) Final product involving many printing steps.
© U. Durig

is crucial in battery, photovoltaic and medical applications, for example. Further development is needed on nano-(and micro-) structuring of surfaces by using green chemistry and dry techniques (e.g., spray, evaporation, chemical vapour and atomic layer deposition), for surface generation and treatment. Additionally, self-assembly/self-organisation processes should be developed for the preparation of highly organised structures. Particular aspects are the design of building blocks, the creation of the proper conditions for assembling, the ability to prompt the system to start working and to dismantle it at the end or to transform its function. Such surface functionalisation and structuring should be correlated with properties and performance, including durability. Examples here are anti-microbial, anti-biofouling surfaces which are efficient in the operating medium (seawater, air-conditioning circuits). (Nanostructured) membrane technology is another poorly understood topic, yet it is of immediate practical importance, e.g., for fuel cells. In a complementary perspective, nanoparticles have entered the industrial landscape predominantly in the form of surface coatings. An illustration of this is titanium dioxide particles with diameters in the range from 20 nm to 100 nm which are used in inkjet printer paper and are produced in ton quantities per day. However, processing of large quantities of nano objects (e.g. nanotubes) with narrow, controlled specification still remains a short-term issue. Nanoparticles placement is another important topic. Here the challenge is the deposition and anchoring of nanoparticles at arbitrary positions with nm accuracy and high throughput and yield. Guided self-assembly from solution has been researched over the past few years. The method works well for spherical particles with a diameter in the range from 20 to few hundred nanometers. However, no solution is known to date even on the conceptual level for the accurate placement of small particles such as quantum dots or aspheric particles such as, for example, carbon nanotubes. The precise and dense packing of carbon nanotubes is one of the cardinal problems to solve for using these materials in high speed switches. The precise placement of quantum dot particles, for example in resonant optical cavities, forms the basis for integrated non-linear optical devices and eventually for studying novel quantum gate structures. This field still requires a substantial amount of basic research on the conceptual level.

- MatSEEC recommends the development of green chemistry and dry techniques for the processing of materials with micro- and nano-structured surfaces.
- MatSEEC recommends that materials and process characterisation techniques should be supported, both at the large instruments level and at that of R&D in the laboratory scale.

4.2 **Analytical Tools**

Characterisation of advanced materials, and particularly of materials with necessarily complex structures such as bio and functional ones, requires analytical tools for observation and monitoring all relevant length scales (nano, micro, meso and macro). Moreover, detailed insight in the matter through analytical tools beyond the state of the art will be an invaluable contribution to the modelling of the structure-properties relationship and therefore to understanding, controlling and monitoring properties and performance of materials, devices and systems (Figure 12). Such tools should demonstrate high spatial resolution and ability to follow the behaviour of the material systems in time. In this perspective, recent progress has been made on synchrotron-based methods with respect to *in situ* capabilities as well as nanofocusing, pushing the spatial resolution further into the nm range. Analytical tools should be able to operate *in situ*, in an operating environment involving, for example, high pressure or living organisms. Surface analysis is a particular field requiring appropriate analytical tools using ultrahigh vacuum electron microscopy and also very low energy modes of the electron microscopy and spectromicroscopy. Free Electron Laser (FEL) facilities have emerged as a novel scientific tool and should be developed for detailed structural analysis at timescales down to femtoseconds. Furthermore, materials processing requires *in situ* analytical tools, which contributes to

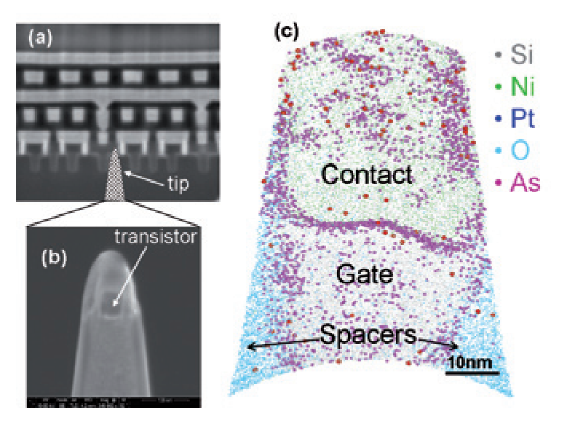

Figure 12. Analysis in 3D and at the atomic scale of a MOS transistor by atom probe tomography (APT): A transistor has been extracted from SRAM memories (a) using focused ion beam and shaped into a tip (b) to be analysed by APT (c). In (c), the atoms drawn as points define the transistor parts: contact (NiSi), gate (poly-Si) and spacers (SiO2). The arsenic atoms (dopants) have been enlarged to show the segregation at the NiSi/Si interface that changes the electrical properties.

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the optimisation of the process itself (by providing process modelling with reliable data) and also to the processing-structure relationship. There is a crucial need for the combination of local tools, facilities and infrastructures as well as large facilities. It is worth recalling here the pan-European effort to produce a comprehensive inventory of research infrastructures of major relevance in Europe across all scientific domains. This project, entitled Mapping of the European Research Infrastructure Landscape (MERIL), is accessible to the public through an interactive online portal.[6] In a complementary perspective, the European Strategy Forum on Research Infrastructures (ESFRI) has been established with the mission to facilitate multilateral initiatives on research infrastructures. The intention is to achieve a better use and development of infrastructure.

MatSEEC recommends facilitating the invention of new analytical tools. Such tools will provide new insights to more refined material control. Progress in analytical tools is needed both in individual laboratories and in small groups as well as at large scale facilities.

4.3 Combinatorial Chemistry and High Throughput Materials Science and Engineering

There is a lack of available extended materials libraries with well identified processing-structure-properties (and performance) relationships with regard to the huge number of the available possibilities.[7] This situation is strongly antinomic with today's societal needs, requiring beyond the state of the art technologies and materials solutions. Meeting such pronounced societal needs involves either incorporation of new functionalities into 'classical' materials (ceramics, metals, textiles, paper, building and construction, etc.) to give them a higher added value, and/or identification of new materials with original properties or multifunctionality. Taking into account that (i) variety is high, (ii) opportunity is high, (iii) probability of finding the best solution is low, and (iv) sampling and screening process is time consuming, such requirements are incompatible with the 'one at a time' methods that are mainly used nowadays. Although well established, a further application of these methods is expected to lead to slow innovation rates, and to expensive, time- and resources-consuming processes. Hence, a solution must be found to overcome the problems related to the number of possible combinations of ternary and higher order systems and to the subsequent extended fields of properties to be explored, managed, mined and modelled. Alternative routes to meet the need for high throughput screening of complex systems has been provided by the pharmaceutical and biotechnology industries. In these fields, automation of the fabrication of specimen arrays, screening techniques and informatics have hastened the development of important new drugs and genetic therapies, which accounts in part for the biotechnical revolution now in progress. Combinatorial, high throughput processing of materials of variable composition, screening of their (micro-)structure and properties, and efficient solutions for the storage, the management and the mining of data libraries are requested (Figure 13). The need for detailed data libraries is

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[6] http://portal.meril.eu/converis-esf/publicweb/research_infrastructure/3395

[7] An illustration of the huge number of possibilities which remains unexplored is that with approximately 80 metallic elements available, one expects more than 6,000 binary systems, and at least 500,000 ternary and 40,000,000 quaternary ones. Up to now, not all binary systems and less than 8,000 ternary ones (not to mention quaternaries) have been looked at crystallographically but, with the exception of a few cases, there is no information on their physical and chemical properties. Corollary to this context, ternary or quaternary alloys in which three or four components, at comparable quantities, determine the basic properties (e.g., the precipitate-hardened nickel alloys) are only scarcely used in metal-based industries.

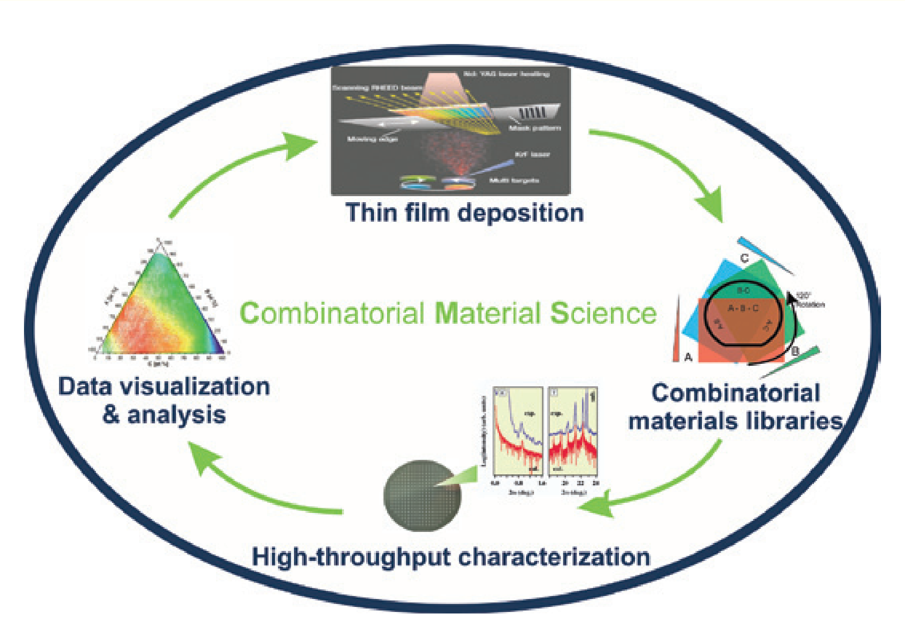

Figure 13. Thin film combinatorial materials science is based on fabrication of materials libraries by special (sputter) deposition processes. Binary, ternary as well as large fractions of quaternary materials systems are fabricated in a single experiment. Libraries are characterised by high throughput methods in order to determine efficiently compositional, structural and functional properties. The resulting data is visualised, e.g., in a ternary composition triangle. Colour coding helps identify regions of interest, which can be investigated in more detail in a 2nd combinatorial cycle.

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coherent with the increasing performance of modelling tools which requires stronger and faster experimental validation.

MatSEEC recommends the support of high throughput activities which will aim at developing easily accessible materials and properties data banks.

4.4 **Modelling**

Progress is needed in developing modelling with predictive power for the processing, structure control and function of advanced materials. This requirement is compatible with the previously mentioned need for ramping up the experimental, high throughput activities providing large quantities of data (both on existing materials and on new classes of materials) to feed modelling and simulation. Modelling is necessary for engineering design and applications (materials by design); it remains a major challenge for highly complex materials such as bio and functional ones. Particular aspects requiring special focus are multiscale modelling, including Quantum Dynamics (QD), Finite Elements (FE), scale transition methods, simulation of processes, reverse modelling. Materials modelling and simulation opens the perspective of achieving novel designed materials, which will naturally have complex structures at different dimensional scales and will therefore be multifunctional. A more comprehensive development of the contribution of modelling and more precisely of computational materials science to future materials and challenges is provided in the *ad hoc* science position paper elaborated by MatSEEC.[8]

One of the greatest challenges in computational materials science is the ability to design a new material to match the required properties for a targeted application. This can be efficiently met by a thorough understanding of how atomic, molecular and mesoscopic features influence macroscopic behaviour, and how properties may change with composition, temperature and pressure. *Ab initio* electronic structure theory of 'real materials' aims at understanding materials properties from an atomistic quantum-mechanical point of view, retaining the complexity of real materials, without losing track of the basic laws of physics. It is now possible to quantitatively design thermodynamic properties and phase transitions in materials from *ab initio* calculations and thereby connect microscopic chemical degrees of freedom with macroscopic behaviour and phenomenological theory using either statistical mechanics or the CALPHAD methodology. Such an approach is illustrated in Figure 14 which compares the calculated Ni-Nb phase diagram with experimental data.

Improvements in the accuracy of *ab initio* methods and developments of new coarse-graining techniques should allow further application of such *ab initio* frameworks as computational modelling

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[8] ESF (2011) *Computational Techniques, Methods and Materials Design*. Niemen, R., ed. Science position paper. MatSEEC, European Science Foundation, Strasbourg. ISBN: 978-2-918428-38-1.

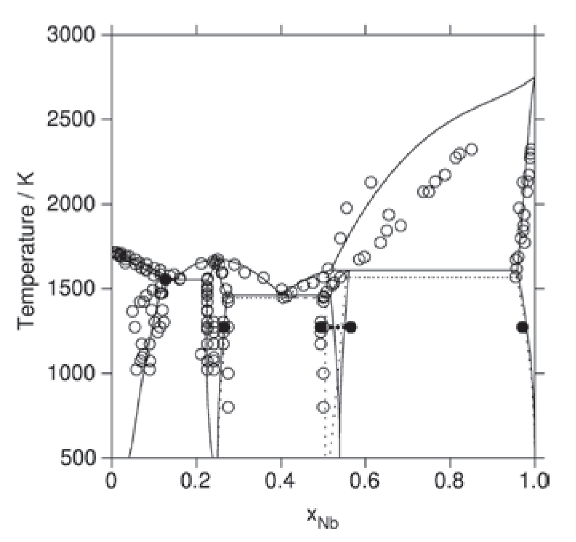

Figure 14. Calculated Ni-Nb phase diagram vs experimental data. © A. Pasturel

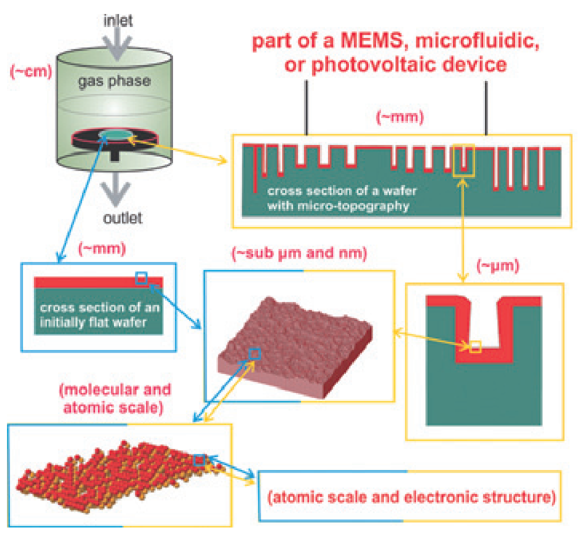

Figure 15. From the reactor's operating valve to the molecular structure of the material. © A. G. Boudouvis

tools of utmost importance in materials science. In particular, by predicting the properties of a series of materials prior to their synthesis, computational modelling can guide experiments in promising directions, and just as importantly, steer them away from attempts that would be less fruitful.

The next challenge in computational materials science is the design of processes giving over the desired, strict specifications for the material properties or system/device behaviour in the micro- and nanoscales that up till now were hard or even impossible to access. Given that the primary manipulation of the events at these scales occurs at the macroscale, a great challenge for multiscale modelling of materials processing emerges: It is the link of the operational (macroscopic) parameters of the operating reactor to the materials properties at the micro- or nanoscale or in other words: *From the reactor's operating valve to the molecular structure of the material.* This multiscale concept is illustrated in the cartoon of Figure 15 for the case of a chemical vapor deposition reactor.

To cover all scales, a multiscale computational framework should be able to perform electronic structure, molecular dynamics, kinetic Monte Carlo, and continuum model calculations. The modelling effort should tune bottom-up (from the smaller to the larger scale) and top-down (from the larger to the smaller scale) approaches to meet at the scale of interest, i.e., micro- or nanoscale. Parallel processing, both with central processing units (CPUs) and graphics processing units (GPUs), is critical to face the challenge of multiscale process simulation.

MatSEEC recommends the development of multiscale modelling fed by large data banks and aimed at (a) optimisation of materials processing techniques and (b) establishing the materials by design approach. It also recommends the development of systematic approaches to verification of the simulation results and the development of error estimates of the computationally predicted properties. It finally recommends facilitation of the networking among the numerous research groups operating in this field.

4.5 Recycling and Availability of Natural Resources

Critical raw materials for Europe have already been compiled in a report edited by the EC, and technological and societal challenges concerned by sustainable mineral resources and by critical elements in particular are addressed within an *ad hoc* European Technology Platform (www.etpsmr.org). Both ceramic and metallic materials are concerned by the availability of critical elements (rare earths, platinum group metals, niobium, tantalum and others).

As materials design becomes increasingly complex to meet the needs of advanced applications, we also rely on a wider spectrum of elements, some of which are either very scarce as a natural resource or difficult to access in a sustainable way for geopolitical reasons. While developing new technologies to reduce our reliance on fossil fuels, we have created a need for rare elements. For example, tellurium

(Te) is used in solar panels and is an important component in thermo-electrics, terbium (Tb) is used in compact fluorescent lighting, and indium (In) is an essential component in transparent conducting oxides used in a variety of optoelectronic devices, including solar cells. Those three elements are only some examples where demand will exceed supply in the near future. Rare earth elements, critical in most permanent magnets, have also suffered from a well-publicised increase in price. There are various origins to the problem of poor supply – ranging from a low natural abundance, a low element concentration, the difficulty in mining and isolation, and the control of the supply chain by few producing countries. These issues can be mitigated by several strategies. First, recycling needs to be improved – for example, gold is more abundant in electronic goods than in ores, yet only 15% is recycled through that route. This strategy is gaining increasing traction through 'urban mining'. As a corollary, materials should be designed with the easy extraction of the rare elements in mind. A counter example is terbium which cannot be extracted from bulbs, because of its combination with the toxic element mercury. Second, where the scarcity of natural resources is confirmed, materials scientists and engineers should find alternatives to replace the element(s) at risk. Third, when developing new technologies and improved materials, consideration should be given to the availability of the component elements, while also acknowledging that low availability might only be due to small demand, and that mining processes can be developed to meet the industries' needs, albeit with some delay. Fourth, more relevant to the supply chain, the efficiency of element mining should be optimised, with the training of a suitable workforce of chemists, engineers, theorists, solid state physicists and geologists, amongst others. The success of efficient use of rare elements relies on transparent communication between all levels of the chain – from production to devices via the creation of new materials and the ease of recycling. It is the responsibility of governments to ensure that the data is available and that funding is adequately directed to exploratory research and training.

Bio-based materials are a very promising source of sustainable structural and functional materials that have the potential of supplementing/replacing currently used metals and oil-based polymers. Biotechnology, including genetic engineering of microorganisms, has the potential of supplying novel structural, functional and multifunctional materials. Nevertheless, the current available bio-based materials have a very limited span of properties, and the development of large-scale production of advanced bio-based materials, with an enriched set of properties, will require a long-term strategic investment in research and development. Biological materials are in general formed and include planned obsolescence and re-use. Bio-based materials, which are envisaged to be carbon-based, have the potential of being designed with an appropriate end-of-life application.

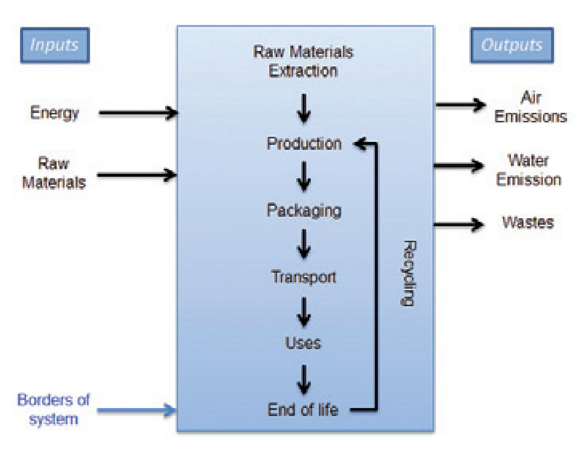

Figure 16. Life cycle analysis.
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The design process in industry, particularly in the chemical industry, is now changing. The holistic challenge of reducing environmental impacts at each stage of the manufacturing process must now be answered. The eco-design of product or process must be integrated. In this approach, the life cycle analysis (LCA, Figure 16) facilitates understanding and quantification of the ecological and human-health impacts of a product or system over its complete life cycle.[9] LCA becomes a strategic tool for innovation by identifying potential for progress in terms of environmental impacts, and energy and resource consumption. This tool makes it possible to direct the efforts of research and development leading to the identification of innovative solutions with lower environmental impacts, to lead to new products, more 'green', eco-designed, meeting the demands of increasingly pressing market and regulation.

The life cycle analysis is actually a method of analysis which quantitatively evaluates all potential environmental impacts of a product or service by considering the entire life cycle. This analysis applies to the entire life cycle in a 'from cradle to grave' approach, insofar as at each stage of the life cycle there is energy and resources consumption,

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[9] UNEP (2013) *Metal Recycling: Opportunities, Limits*. Report 2b of the Global Metal Flows Working Group of the International Resource Panel of UNEP, 2013

and generation of environmental, social and economic impacts. This analysis is based actually on four well-defined phases: defining the objectives and the scope of the analysis of life cycle; the inventory of the life cycle; the impact evaluation of the life cycle; and, finally, the interpretation of the life cycle. The analysis is based on a scientific methodology, which relies on computer software, framed by the ISO 14040 and 14044. The life cycle analysis is therefore to assess, within a system defined by borders, the impacts due to incoming – consumption of natural resources – and to outgoing – emissions in the air, water, soil and other nuisances.

MatSEEC recommends that funding should be directed at developing strategies for more efficient use of natural resources, both by the development of alternative materials and the improvement of recycling routes.

4.6 **Interdisciplinarity**

It appears obvious that MSE maintains strong links with other fields of research and technology development and for this reason is highly complex. This is particularly illustrated in the case of biomaterials and nanotechnology. It has also an increasing impact on the novel approaches and future challenges of the family of advanced classics such as metals, ceramics and polymers. Figure 17 illustrates an example of the strongly interdisciplinary character of MSE. In this scheme, a significant advance or discovery in Discipline C combined with input from Disciplines A, B and D is assimilated within MSE and allows materials to be tuned in order to overcome a barrier of the societal challenge 'energy'. Here, the term 'discipline' refers both to scientific and to technological domains. In this perspective, the further we move into the future, the more the contribution of MSE is diluted within required progress in other domains. Inversely, MSE can 'guide' the basic disciplines: we request from coordination chemistry to design a molecular compound which can respond to the specifications of a precursor for chemical vapour deposition… The solution to these problems provides products, processes and services which are beneficial to the industry as is illustrated in the figure by the red lines. Concrete examples for this situation are the design, processing and evaluation of catalytic materials, and hybrid materials such as composites consisting of one inorganic and one organic constituent at the nanometer or molecular level.

This increasing interdisciplinary nature of MSE implies that it is not recognised as a field of its own, as it is lumped together with other topics. This results in difficulties in managing scientific programmes and in evaluating professional careers.

MatSEEC recommends separate evaluation panels dedicated to materials science and engineering, rather than having materials as a subset of physics or chemistry panels, reducing the chances of the referees appreciating the crucial role of materials research in broad research programmes.

4.7 **Funding**

In general, MSE is not recognised as a field of its own, as the field is aggregated with other topics. Among the consequences of this situation is that evaluation of MSE projects is often attributed to peer review

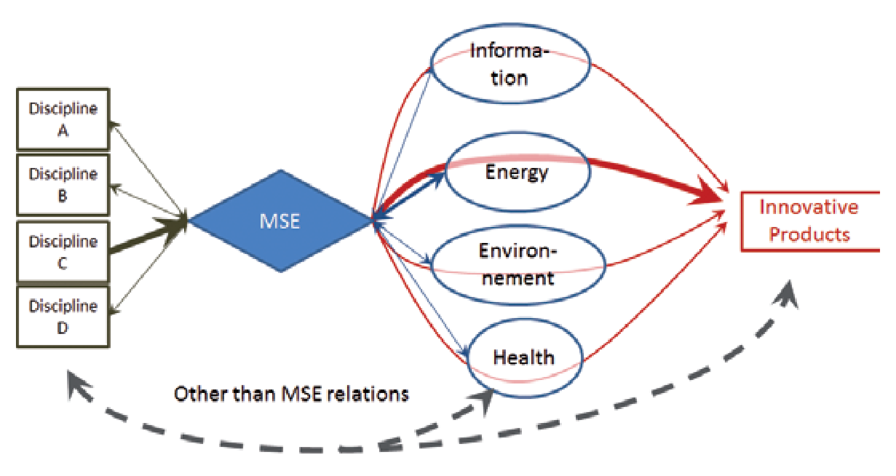


Figure 17. Strongly interdisciplinary character of MSE.
© C. Vahlas

panels which are also in charge of evaluating other, more established disciplines incorporated into the proposals (e.g. chemistry and materials). Also, grant proposers must trust to chance that a proposal is judged by competent reviewers, or even reviewers who are sensitive to the importance of the field of materials science and engineering and the challenges faced in the development of suitable materials.

EU support to pre-competitive research has been successful in the recent past. Nevertheless, there exist no workable schemes for funding of bottom-up basic research across national borders. Schemes based on cooperation of national funding agencies are too complicated and inefficient, and discourage most laboratories searching for the optimal partner within EU but outside their country to set up collaborations. This is a typical handicap of the EU, which does not exist in the USA. The lack of public funding for pre-competitive research leads groups to enter into collaboration with (a single) industrial partner at a very early stage. Considering IPR issues, this is perceived as a major constraint in setting up open collaboration, maturing the knowledge and making new techniques and products available. It may also channel the resulting IPR actually out of the EU, as local industries often have their corporate headquarters outside the EU. Advance with respect to other regions worldwide will be lost soon if efficiency of support of exploratory research is not improved.

- MatSEEC recommends that, in addition to supporting pre-competitive research, European funding agencies should continue supporting exploratory research so as to maintain Europe's strength in academic research.
- MatSEEC recommends the creation of a dedicated ERC peer review panel for Materials Science and Engineering.

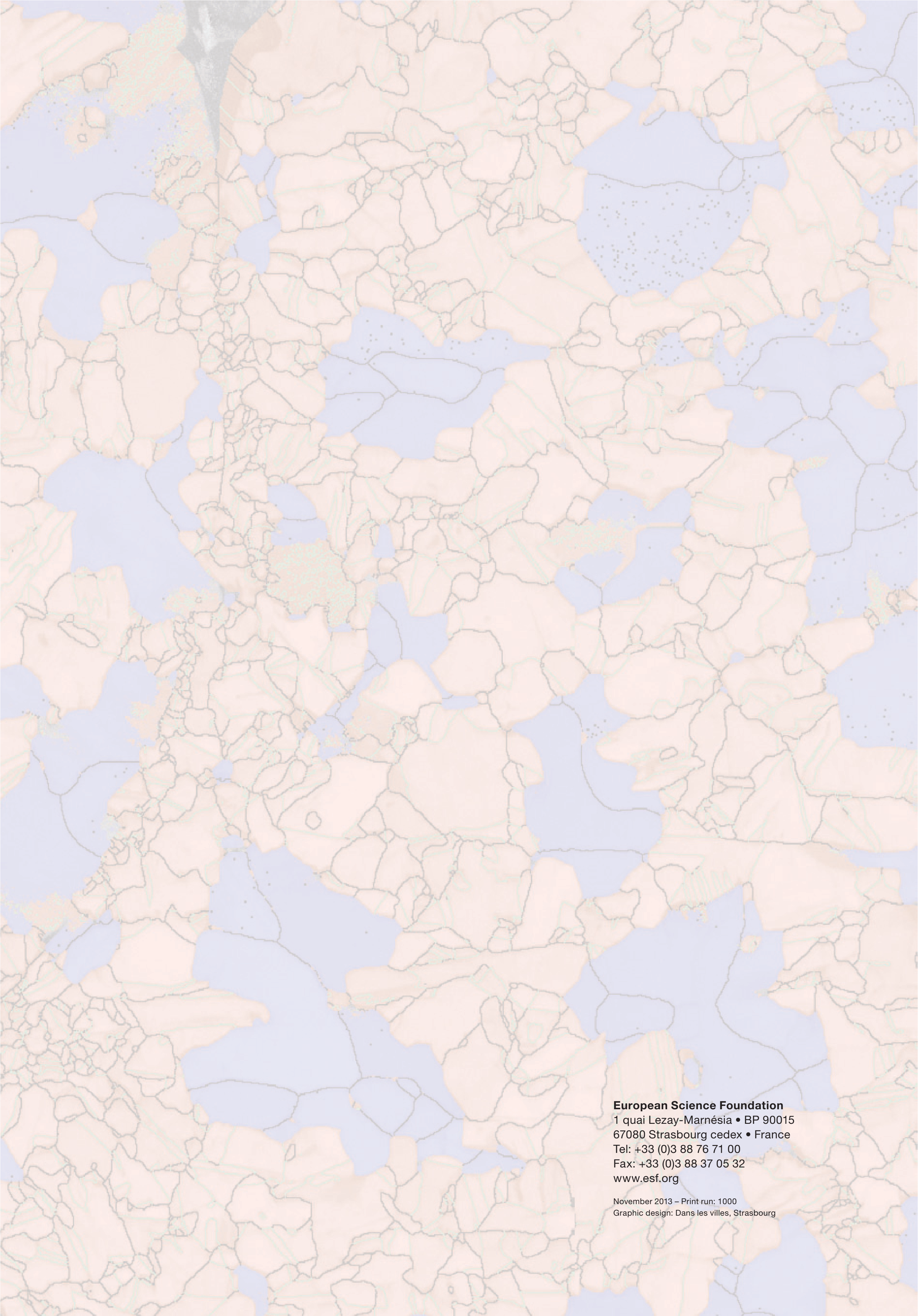
4.8 **Education**

Training for a career in MSE is recognised as a challenge that will affect our ability to attract the most qualified workforce to materials research and technological development. Training starts at the undergraduate (UG) level where MSE as a subject has a poor visibility or reputation compared to traditional disciplines in sciences (chemistry, physics, biology) or engineering (civil, mechanical, electronic, etc.). In some countries it is not even offered as a subject of studies. This is most probably due to the interdisciplinarity of the subject, which is why some students might consider it as superficial. We need to work to change perception amongst students that interdisciplinarity should be intimidating due to its open-endedness, but rather an opportunity to learn and achieve more. This could be done via outreach efforts at universities, more prominent showcasing of what progress can be achieved thanks to materials, showcasing of successful role models (http://archive.sciencewatch.com/dr/sci/misc/Top100MatSci2000-10/), efforts of popular science programmes, or regular features on reputable news websites (http://www.bbc.co.uk/news/science-environment-20084285). The results are yet to translate into increased numbers of UG applications as, especially in a more precarious economic climate, students will favour traditional disciplines.

At the postgraduate (PG) level, materials-centred projects can be realised by UGs trained in disciplines outside MSE, and we may benefit from the influx of different expertise. It is, however, important that common ground should be found, and therefore a format of a more structured PhD, which includes a masters centred on a specific materials discipline (e.g., nanomaterials, functional materials, biomaterials, etc.) and including courses is recommended. Recognising the high demand for materials graduates in industry, it will be particularly important to engage with industrial partners to include some practical experience outside the academic framework.

It is also important to explore new approaches to advanced education in interdisciplinary topics that bridge classical disciplines, (bio-) engineering, materials and computer sciences.

- MatSEEC recommends that a balance of industry efficiency and academic creativity is established for future industry.
- MatSEEC recommends that advanced education should explore new approaches in interdisciplinary topics in order to create bridges between classical disciplines, (bio-) engineering, materials and computer sciences.



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