madrid institute
for advanced studies

imdea

Scientific Program (2008-2011)

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SUMMARY

1. BACKGROUND

1.1. Context

The "Instituto Madrileño de Estudios Avanzados en Materiales" (IMDEA-Materials) (Madrid's Advanced Studies Institute of Materials) is one of the new research institutes created by the Regional Government of Madrid as part of IV Regional Plan for Scientific Research and Technological Innovation. The new research institutes of Madrid are to provide a new institutional framework that combines both public and private support to science and harmonizes research with market demand, encouraging the private sector to participate in the design of science.

The general objectives of the new institutes – defined by the Comunidad de Madrid in accordance with the IV Regional Plan for Scientific Research and Technological Innovation – are the following:

- Research of excellence in the selected field
- Technology transfer to the industrial sector to improve competitiveness.
- Agility to obtain funds from several sources
- Recruitment to internationalize the research in the region of Madrid.

To achieve these goals, IMDEA-Materials has been provided with a legal and organizational structure detailed in other documents. This report justifies and develops the scientific program and the main research lines that will drive the Institute's activity during the next five years.

1.2. Materials Research in Madrid

To evaluate the potential of the research groups of Madrid in the materials, a meeting was arranged with the directors of the research institutes and of the materials departments from the Universities of Madrid that had obtained

funding in the call "Programas Conjuntos de Actividades de I+D de la CM". The meeting was held at the Department of Materials Science (Polytechnic University of Madrid) on December 13th 2005. Over 30 people attended in representation of thirteen materials departments and research institutes in the region of Madrid. The basic conclusions of the meeting can be summarized as follows:

- The region of Madrid has a high scientific potential and excellent infrastructure in Materials Science and Engineering. The R&D in this field is wide, intense and varied and the Institutes and Departments represented at the meeting have demonstrated their ability to carry out basic research of high quality, judging by the results (publications, research funding obtained in competitive national and international programs, etc.). From this point of view, Madrid has the necessary human capital to create the new IMDEA-Materials. A weak point in the research capacities in Materials Science and Engineering in Madrid might be the imbalance between the numerous groups and resources devoted to the characterization of the properties and the relatively scarce means devoted to the processing of new materials and development of components, particularly at a pre-industrial or pilot-plant level.

- The need of academic and professional training in Materials Science and Engineering is well covered in the region of Madrid: Three universities give the Materials Engineer Degree and two others have a speciality in Materials as part of another degree. Furthermore, universities and some CSIC research institutes give postgraduate, specialization or master courses in the materials area.

1.3. Current Industrial Panorama

To investigate in depth the significance of the materials sector, a study of the "Industrial reality of materials in the region of Madrid" was commissioned from the "Círculo de Innovación en Materiales, Tecnología Aeroespacial y Nanotecnología" of the Carlos III University of Madrid. The main conclusions

of this research are presented in the following lines as relevant to the selection of the research lines of IMDEA-Materials.

- Materials do not constitute an industrial sector of economic activity; they are rather transversal to it. Several sectors use, design, manufacture and generate wealth with materials. If we consider only the industrial activity related to the classic materials –metals, polymers and ceramics– and include the industrial activity of materials integration into structures, devices or systems, recycling and materials testing, the materials sector comprises around 12.000 companies, that employ about a half a million people and whose business volume is about 150.000 million euros.

- The business world is fairly well structured. Some 49 business associations were found in the sectors of metallic, ceramic and polymeric materials, 9 associations in the materials integration sector, and 30 in the rest of the sectors. 86 companies were identified in the region that carry out research activities and invest part of their working capital in innovation. 35 of these 86 companies with R&D activities in the field of materials have applied for grants from national research projects and this shows the gap between basic and applied research and the industrial fabric.

The study selected 29 large- and medium-sized enterprises strongly positioned in the region of Madrid which carry out R&D activities and invest part of their working capital in innovation in the materials sector. Most of these companies belong to the transportation (automotive, aerospace) and construction sectors, and their interests lies in materials with a structural function, although more and more it is necessary to harmonize this function with esthetical and functional requirements that generate the need for multifunctional materials with an essential structural application.

1.4. Conclusions

The general objectives of the activity of IMDEA-Materials and the analysis of the scientific and industrial reality of materials in the region of Madrid lead to

the following conclusions concerning the scientific program of the new institute:

- Basic research activities in Materials Science and Engineering are well developed in Madrid, although the weak point of the research in the region (and generally in Spain) is the transfer of technology to the industrial sector[1]. This task –together with high quality research at international level- will mark the identity of the new institute, which must contribute actively to improve the competitiveness of industry in the materials sector. Furthermore, industrial collaboration will be essential to cover part of the institute's expenses.

- In order to promote the participation of companies in the institute, some of the main research lines are grouped in an area of scientific interest that allows the transfer of technology to industry in the region of Madrid. Together with these applied research lines, the institute will develop other research closer to the forefront of knowledge in Materials Engineering and that will preserve the environment of scientific excellence.

- There must be a critical mass of researchers in the region of Madrid in some of the selected research lines to start the new institute. These researchers will make it possible to start with the Institute activity and channel the progressive incorporation of new researchers following the strategy of internationalization.

- The scientific activities have to be interdisciplinary, and the scope of research wide enough to face medium-term scientific and technological challenges.

From these conclusions, a draft of the scientific program of the Institute for the next four years has been prepared by a task group composed by Prof. Javier LLorca (chair, Universidad Politécnica de Madrid), Prof. Juan Balsega

[1] "Technology transfer" must be understood as the carrying out of mid or long-term (2-5 years) research projects which result in the development of new materials or processes for industrial applications and make it possible to keep the leadership of companies in their sector. This is far from the collaboration (also necessary but different) of technological centres with industry.

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2. RESEARCH LINES

2.1. Selection

The scientific potential in Madrid in terms of quality and specialization makes it easy to identify research groups of international standing in most of the research topics in Materials Science and Engineering, which will be able to nucleate the new Institute. Moreover, it is not difficult to identify research lines in the frontiers of knowledge associated to technological problems of large social and/or economic impact. So the main limitation to select the research lines of the new Institute is to find topics which will facilitate the transfer of technology to Spanish enterprises while maintaining the scientific character of the Institute, very different from that of technological centers which provide specialized services for industry.

From the viewpoint of the transfer of technology, a fundamental issue is to focus several of the research lines of IMDEA-Materials on the mid- and long-term priorities of industrial enterprises which have shown a serious commitment to research and development activities in the past and which are willing to collaborate with the Institute in their development. This will guarantee the industrial exploitation of the new developments and help to provide financial support for the Institute through contracts with industry and participation in national and international research programs. 29 large and medium Spanish industrial enterprises which carry out R+D activities on materials (identified in the analysis of the industry mentioned in the previous section) were approached about their interest in collaborating with the Institute within the following framework:

- The industrial companies will benefit from the human capital and the research infrastructures provided by IMDEA-Materials for research along lines of primary interest for the mid- and large-term development of new materials and components.

- The goals and the aims of the research lines proposed by the industrial partners have to incorporate scientific and/or technological challenges beyond the current state-of-the-art.

- The industries will establish a partnership with the Institute to develop these research lines and will contribute to cover part of the research costs either directly of through participation in national and international research programs.

- The industrial partners will be represented on the Board of Trustees of the Foundation.

Five companies (Grupo Antolín, Industría de TurboPropulsores, Aries-Complex, Gamesa and Tolsa) agreed to participate. The research interests of four of them were focused on the development of new materials and components for structural applications for the automotive industry (Antolín), gas turbines (ITP), aerospace (Aries-Complex) and aerogenerators (Gamesa). The fifth one, Tolsa, is one the largest suppliers of nanoclays (mainly sepiolite) worldwide and is looking for new applications for these materials in different sectors.

The research interests of these companies expose the current situation of the industrial R&D in materials in Spain. Basically, the number of industries that can benefit from scientific and technological developments carried out by the Institute in the area of functional materials (microelectronics, magnetic and optical materials, superconductivity, etc.) is very limited, but some companies are interested in the development of new materials with improved properties for structural applications in the aerospace, automotive and energy sectors. In addition, materials application often requires nowadays the integration of various purposes (esthetic, mechanical, biocompatibility, information transfer, etc.) and this has led to the development of multifunctional materials in which the structural function is integrated with other functionalities.

Thus, two main research areas proposed for IMDEA-materials. The first, more applied, and encompassing the mid-term research interests of the companies associated with the institute, will deal with the processing techniques, design and application of advanced structural materials in the aerospace, automotive and energy generation sectors. As shown below, these interests are focused around two main types of materials: advanced metallic alloys and structural composites. Key materials and technologies of current interest to the companies are identified in the scientific program, but the expertise and the equipments can be easily transferred to research in other materials of the same class.

The second main area will cover topics in the forefront of scientific and technological research which are linked to the previous one and that will help to support the previous activities and to provide long-term technological leadership. The activities included in this second area will include the development of hybrid structural materials or multimaterials on different scales of integration, smart materials (whose structural function is supported by sensors and actuators), tailored materials (including biomimetics, microstructural optimization, self-assembly) as well as the application of sophisticated simulation techniques (modeling of materials processing, properties and in-service reliability), eliminating the costly trial and error strategy which has been standard so far for the development of new materials.

2.2. Structure

Research in Materials Science and Engineering has always been located in the middle of a tetrahedron whose vertices are Processing, Properties, Modeling and Application. This means that this scientific discipline is by nature multidisciplinary and requires the expertise from these four different areas. This will be translated into the structure of the IMDEA-materials, which will be organized along vertical and transversal research lines. The vertical research lines will include processing and application and will be focused on the development of new materials and components working in close connection with the industrial partners to cover the demands and requirements of the market. They will be organized according to the different types of materials,

whose processing and requirements are normally different. Horizontal lines will cover the properties and modeling vertices of the tetrahedron and will provide expertise in common areas which are necessary for the development of materials (characterization, simulation) and in which the expertise needed is similar for the different types.

The Institute will begin its activities with 7 research lines, whose main characteristics and goals, and their links with industry, are described below. This number will be increased progressively up to 10 (and approximately 100 researchers) taking into account the scientific and technological results obtained and the new challenges and industrial partners which join the Institute in the future.

2.3. Vertical Research Lines

In agreement with the research interests of the industrial partners, IMDEA-materials will begin its activities in two main areas (*advanced metallic alloys* and *structural composites*), which will include four research lines:

2.3.1. *Metallic Alloys for High Temperature Structural Applications*

This line is strategic for Industria de Turbo Propulsores S. A., manufacturer of gas turbines mainly for aerospace applications. Technological leadership in this sector is based on improving the efficiency and the reliability of materials and components, and this requires the development of new structural materials with an optimum combination of mechanical properties at high temperature in aggressive environments for long periods of time. In addition, low densities are always at a premium in aerospace applications.

The objectives of this research line will include:

- The improvement of casting technologies (vacuum and inter atmosphere, regular and centrifugal) for high temperature Ni/Co-based superalloys and intermetallic compounds.

- The production of near net-shape components of these materials from powders using conventional powder metallurgy techniques, hot-isostatic pressing, and novel methods based on rapid prototyping, electron-beam melting, direct-metal laser-sintering, etc…

- Processing and characterization of thermal-barrier and antifriction coatings to improve the durability and structural integrity of critical components.

2.3.2. *Light Metallic Alloys*

High fuel prices in the foreseeable future will act as a driving force to reduce weight in transportation, and foster the use of metallic alloys based on light metals (Al, Mg, Ti). This long-term challenge has led to Grupo Antolín S. A. to open in 2006 a new plant of Mg casting to provide components for the automotive industry, and the group is committed to expand these products in this and other sectors (railways, aerospace). IMDEA-materials will help the industry in this enterprise by helping to achieve the following objectives:

- New Mg alloys for casting with improved mechanical properties and corrosion resistance.

- Viability of new processing techniques (forging, extrusion, thixoforming) to manufacture near neat-shape components.

- Development of modeling tools to simulate the processes (casting, forging, injection) including the microstructural development after solidification.

- New metallic alloys and intermetallic compounds with improved specific properties.

2.3.3. *Structural Composites*

Gamesa, manufacturer of wind-mills, and Aries-Complex, supplier of components for the aerospace industry, are major producers of these

components made of structural composites given the outstanding mechanical properties of these materials in terms of specific stiffness and strength. Key areas for maintaining their industrial leadership in this area are:

- Improvement of current manufacturing techniques (pultrusion, RTM).
- Development of composite materials for high temperature applications and of new composite material systems.
- Composite-composite and metal-composite joints with high reliability and strength.
- Simulation of the mechanical performance of composite materials and structures. Virtual testing.
- Smart composites.

2.3.4. *Nanocomposites*

The dispersion of nanometric reinforcements in polymeric, ceramic and metallic matrices has led to a new class of materials named nanocomposites with unexpected mechanical and functional properties, and constitutes one of the frontiers of knowledge in Materials Science. The Institute will join the current research effort in this area and will collaborate in this line with Tolsa, world leader in the production of sepiolite, a fibrous clay of nanometric dimensions. Tolsa is committed to find new applications (and, thus, new markets) for nanocomposites based on nanoclays and is pursuing various research lines in which IMDEA-materials could help. The main research activities of the Institute in the line will include:

- The development, characterization and simulation of nanocomposite materials with improved mechanical properties and integrated structural and functional capabilities.

- Modification of sepiolite and development of sepiolite-reinforced composites for applications in sensors, catalysis, energy-production systems (fuel-cells) and biocompatible polymers.

2.4. Horizontal Research Lines

Three main horizontal research lines have been identified to provide support for the vertical lines. They will cover the two remaining vertices of the Materials Science and Engineering tetrahedron, namely Properties and Modeling. The techniques and expertise provided by this research are readily applicable to any type of materials and processes. It should be noted that these horizontal lines are designed as actual research lines and not merely as support laboratories. They will work in close connection with the scientists working along the vertical lines to develop new materials and components but they will also have their own research goals in each area.

2.4.1. *Microstructural Characterization of Materials.*

Materials Science was built upon the hypothesis that most of the properties of materials are controlled by the structure on the nm – mm length scales, rather than by the chemical composition. The development of new materials and the improvement of existing ones need a deep knowledge of the microstructure, and this research area has profited in the last decades from huge improvements in the characterization tools, which are essential in any research of materials.

This research will be aimed to provide a state-of-the-art analysis and characterization (qualitative and quantitative) of the composition and microstructure of materials from the atomic level to the micrometer using different kinds of microscopy (approximation, scanning and transmission electron, optical, etc.), spectroscopy, X-ray diffraction and high-resolution three-dimensional computer assisted-tomography, and non-destructive evaluation techniques (ultrasounds, eddy-currents, magnetic particles, etc.).

The cost of all the equipment associated with this research is very high, and it is envisaged that this work will be centered in one research facility in Madrid in which most of the necessary infrastructures are already in place. The equipment and expertise necessary for all the goals enumerated in the previous paragraph will be covered by IMDEA-materials and the facility will have the status of a laboratory associated with IMDEA.

2.4.2. *Mechanical Characterization of Materials*

A materials institute mainly devoted to structural materials needs a research line in the area of the mechanical characterization on different length scales and under different conditions. In particular, it should be able to provide information on the mechanical properties of the microstructure (upon which the relationship between microstructure and properties can be built), to determine the main mechanical properties of laboratory specimens (which are used in standard engineering design), and to establish the behavior of materials under service conditions, which often control the life-cycle and cost.

This research line will provide the Institute with the tools and expertise for the characterization of the mechanical behavior of materials and components, critical to establish the relationship with the microstructure and to establish the in-service performance of the materials developed in the vertical research lines. It will be able to characterize the mechanical behavior of materials at the nm – mm length scales, to determine the mechanical behavior of materials and components under extreme conditions, including different loading conditions (uniaxial and multiaxial, monotonic and cyclic), forces (from mN to MN), strain rates (from quasi-static to ballistic impact), environments (inert or aggressive media, high vacuum or controlled atmospheres, corrosive solutions, etc.) and temperatures (from cryogenic to very high temperatures).

As in the previous research line, given the cost of the infrastructure, one facility in Madrid should be used which already has most of the equipment and expertise. The facility will be a laboratory associated with IMDEA-materials and the IMDEA investment will only supplement the actual expertise and equipment to reach the capabilities indicated above.

2.4.3. *Simulation of Materials and Processes*

The increasing power of digital computers, together with the developments in numerical tools to model physical processes, has led to an explosion in the field of simulation. Behavior that could only be studied by tedious, and often expensive, physical experiments, is now within the grasp of computer simulations. Within the field of materials science and engineering, computer simulations can predict the nucleation and evolution of the microstructure during processing or under service conditions, and provide detailed information of the role played by different physical mechanisms in the deformation and fracture of materials on various length and time scales, which it would have been very difficult and expensive to obtain through experiments.

Obviously, the widespread use of computer simulations will lead to a new paradigm in the development of new structural materials in the future. The classic trial-and-error approach will be substituted by the design of the materials and processes through computer simulations, which will provide optimum microstructure for a given application.

It is believed that a materials Institute committed to research in structural materials in the forefront of the knowledge should include a research line in the area of materials simulation. The expertise required will be focused into two main topics: materials processing (using different tools such as phase-field models, Monte Carlo and phase-diagrams simulations, finite elements, etc.) to determine the influence of processing conditions on the materials microstructure, and multiscale simulations (based on molecular and dislocation dynamics, computational micromechanics, etc.) to predict the macroscopic properties of materials from the properties and spatial arrangement of their constituents. This latter methodology will expand to carry out reliability analyses to assess the behavior of materials and components under service conditions. The computer power necessary for this task is already available in IMDEA.