madrid institute
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biennial report
2008-09

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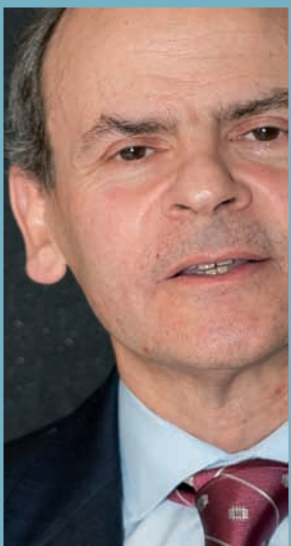
foreword



Javier LLorca
Director IMDEA Materials

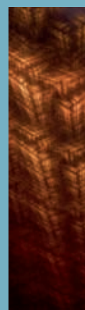
Madrid, December 2009

Sometimes dreams become real. As I begin to write this foreword, I realize that this is precisely what had happened with IMDEA Materials. Its goals, structure, and dominant features were slowly taking shape towards the end of 2005 as a result of the partnership among officials from the Madrid Regional Government, scientists from universities and research centers of Madrid, and leading Spanish companies. A few were committed to succeed, some were sceptical, but most of us realized that this opportunity should not be missed because it could make a difference in the way research in Materials Science and Engineering is carried out in Spain.

With contributions from all of them, IMDEA Materials was born in 2007 with three distinct objectives: excellence in research in Materials Science and Engineering, technology transfer to the industrial sector in order to maintain technological leadership, and attract talent from all over the world to Madrid to work in a truly international and interdisciplinary environment. A small and enthusiastic group started to work on these dreams, looking for talented researchers around the world, launching the first research projects and preparing the provisional laboratory in the space provided by the Polytechnic University of Madrid at the School of Civil Engineering. The provisional site was inaugurated in October 2007, and the first researchers arrived shortly afterwards.

And the achievements summarized in this biennial report show that these dreams became real during 2008 and 2009. IMDEA Materials currently counts with 22 researchers with nine different nationalities (Argentina, Australia, Austria, Belgium, France, India, Spain, United States and Venezuela). They have joined IMDEA Materials after working at prestigious universities and research centers throughout the world, such as Massachusetts Institute of Technology, University of Sydney, Max Planck Institute for Iron Research, Delft University of Technology, Lawrence Livermore National Laboratory, Cambridge University, etc. Leading researchers lead to relevant scientific contributions and IMDEA Materials´ scientists published over forty papers in international peer-reviewed journals, including those with the highest impact in Materials Science and Engineering such as Advanced Materials, Acta Materialia, Physical Review Letters, Journal of the Mechanics and Physics of Solids, etc, and have registered two international patents in this short period. In addition, this expertise and the broad network of international contacts have promoted the participation of IMDEA Materials in twenty research projects, of which seven are international endeavors supported by the framework programs of the European Union. Last, but not the least, IMDEA Materials has attracted the interest of large and small industrial enterprises from Spain and abroad (Airbus, Antolín, Gamesa, Rolls-Royce, Industria de Turbo Propulsores, Intel, Future Fibres, Aries-Complex, Aernnova) which have also funded research programs in areas they consider important to maintain their technological leadership.

A good beginning makes a good ending. I am sure that insofar as IMDEA Materials continues to attract talented people, this proverb will live again.



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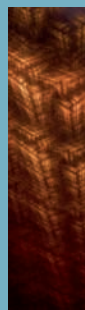


1

general presentation

1.1. Profile

IMDEA Materials (Madrid Institute for Advanced Studies of Materials) is a non-profit independent research institute promoted by the Madrid Regional Government to perform research in Materials Science and Engineering. IMDEA Materials belongs to the Madrid Institute for Advanced Studies network, a new institutional framework created to foster social and economic growth in the region of Madrid by promoting research of excellence and technology transfer in a number of strategic areas (water, food, social sciences, energy, materials, nanoscience, networks, and software).

1.2. Motivation and Goals

The analysis of the research panorama in Materials Science and Engineering in Madrid shows the presence of a number of research groups at universities (Complutense, Autonomous, Polytechnic, Carlos III and Rey Juan Carlos) and CSIC research centres (ICMM, ICV, ICTP, CENIM) with a well-established international reputation and state-of-the-art research infrastructures (mainly for characterization). Nevertheless, this expertise neither resulted in a significant technology transfer to improve the competitiveness of Spanish and European industries nor attracted talent from abroad. These two points are critical to maintain the technological leadership of Spain and Europe; IMDEA Materials was created with an innovative legal status (non-profit independent organization) and a carefully designed relationship with industry (strategic partnership) to achieve these goals.

IMDEA Materials is committed to three main objectives: excellence in Materials Science and Engineering research, technology transfer to the industrial sector in order to increase competitiveness and maintain technological leadership, and attract talented researchers from all over the world to Madrid to work in a truly international and interdisciplinary environment.

1.3. Legal Status and Management Structure

IMDEA Materials is a non-profit independent organization (Foundation). This structure brings together the advantages and guarantees offered by the foundation status with the flexible and dynamic management typical of a private body. This combination is deemed necessary to attain the goals of excellence in research, cooperation with industry and attraction of talented researchers from all over the world.

The main governing body of the Institute is the Board of Trustees. The Board includes representatives of the Regional Government of Madrid (4), universities and research centres of Madrid (4), scientists with an international reputation in Materials Science and Engineering (5) and industrial enterprises (5), together with an independent expert. The industrial enterprises are committed to a long-term strategic partnership with the Institute to develop research lines. The Board appoints the Director, who is the CEO of the Institute, among scientists with a well-established international reputation in Materials Science and Engineering. The Director is assisted by the Deputy Director and the Manager, who take care of the legal, administrative and financial activities of the institute.

The Board of Trustees and the Director are assisted in their functions by the Scientific Council, an advisory board currently made up of 13 scientists from all over the world with expertise in different areas of research covered by the Institute. The tasks of the Scientific Council include the selection of researchers and the evaluation of scientific activities of the researchers and of the institute as a whole to ensure excellence in research.

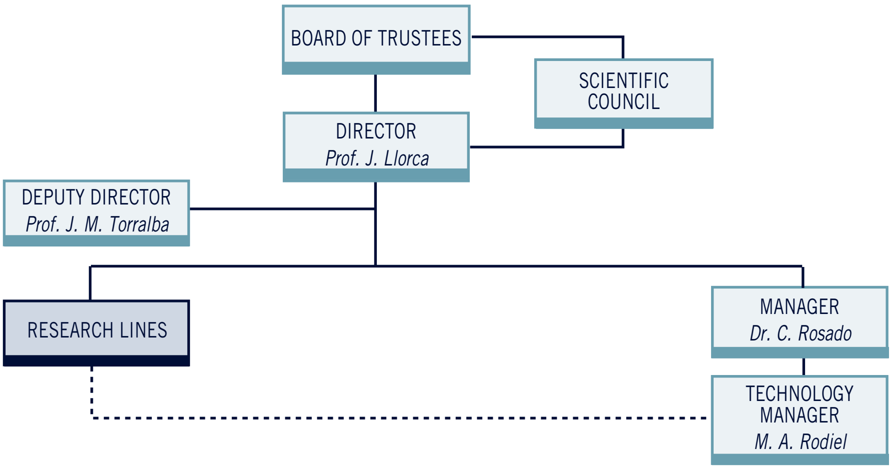


Figure 1. Management structure of IMDEA Materials

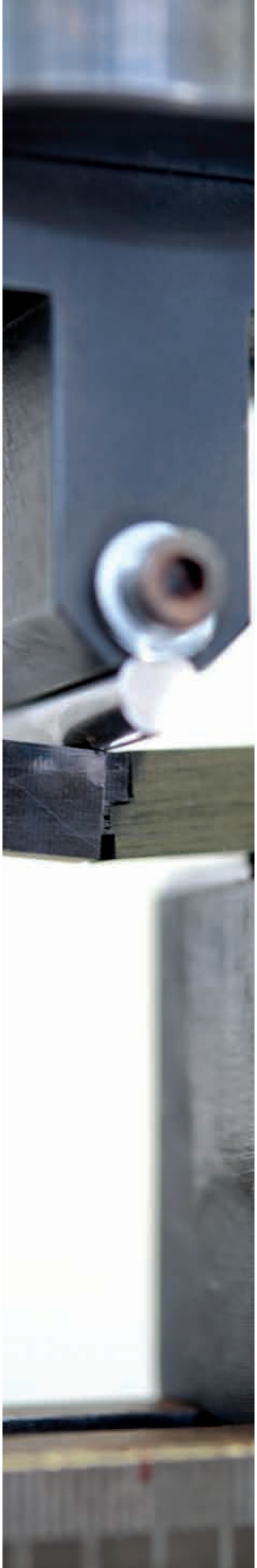
Figure 2. Future headquarters of IMDEA Materials in Tecnogetafe.

1.4. Location

The provisional site of the Institute was inaugurated in October 2007, after refurbishing the space provided by the Polytechnic University of Madrid at the School of Civil Engineering. This site includes 200 m^2 of office space and 140 m^2 of laboratory and currently hosts the offices for the director and staff and the Divisions of Composite Materials and Modelling & Simulation as well as the research line on Nanomechanics and Micromechanics. Another provisional site was opened in September 2009 in premises rented by the Carlos III University to host the Division of Metallic materials and the research line on Multifunctional Nanocomposites. The final site of the Institute will be located at the Technological Park of the Polytechnic University of Madrid in Tecnogetafe. The new building includes over 4000 m^2 of laboratory space and 2000 m^2 of offices to accommodate administrative, technical and research personnel. Construction of the building has already started and it will be available by October 2011.

1.5. Governing Bodies

Board of Trustees



Scientific Council

Prof. Dr. Brian Cantor
Vice-chancellor
York University. England

Prof. Dr. Trevor William Elices
Professor
Cambridge University. UK

Prof. Dr. Manuel Elices
Professor
Polytechnic University of Madrid. Spain

Prof. Dr. Toribio Fernández Otero
Professor
University of Cartagena. Murcia. Spain

Prof. Dr. Randall M. German
Associate Dean of Engineering
San Diego State University. USA

Prof. Dr. Peter Gumbsch
Director, Fraunhofer Institute for Mechanics of Materials
Professor
University of Karlsruhe. Germany

Prof. Dr. Rodolfo Miranda
Director, IMDEA Nanoscience
Professor
Autonomous University of Madrid. Spain

Prof. Dr. Andreas Mortensen
Professor
Ecole Federale Polytechnique of Lausanne. Switzerland

Prof. Dr. Pedro Muñoz-Esquer
Deputy Director
FIDAMC. Spain

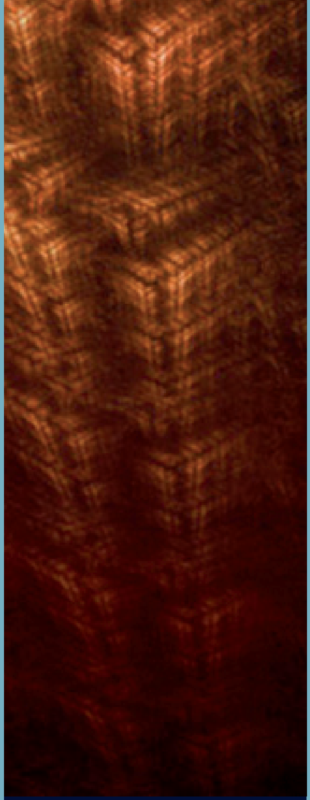
Prof. Dr. Eugenio Oñate
Director, International Centre for Numerical Methods in Engineering
Professor, Polytechnic University of Catalonia. Spain

Prof. Dr. Thomas J. Pinnavaia
University Distinguished Professor
Michigan State University. USA

Prof. Dr. Gary Savage
Director of Operations
Mercedes GP Formula One Team. UK

Prof. Dr. Subra Suresh
Dean, School of Engineering
Massachusetts Institute of Technology. USA

2 research focus



The goals of IMDEA Materials, particularly the excellence in research and technology transfer to industry, require a delicate balance between fundamental and applied research activities. This is obtained by dividing the research focus into "vertical" and "horizontal" lines.

Vertical research lines are focused in new materials and components of interest for industrial enterprises which have established a strategic partnership with the Institute to develop research lines. This association guarantees the industrial exploitation of the new developments as well as the financial support for the Institute through contracts with industry and participation in national and international research programs.

Horizontal research lines establish areas of expertise in the forefront of scientific and technological research that go beyond the state-of-the-art and provide technological leadership looking at the long-term challenges of the industrial partners. The combination of horizontal and vertical lines is expected to establish IMDEA Materials as a leading research institution in Materials Science and Engineering in the international arena.

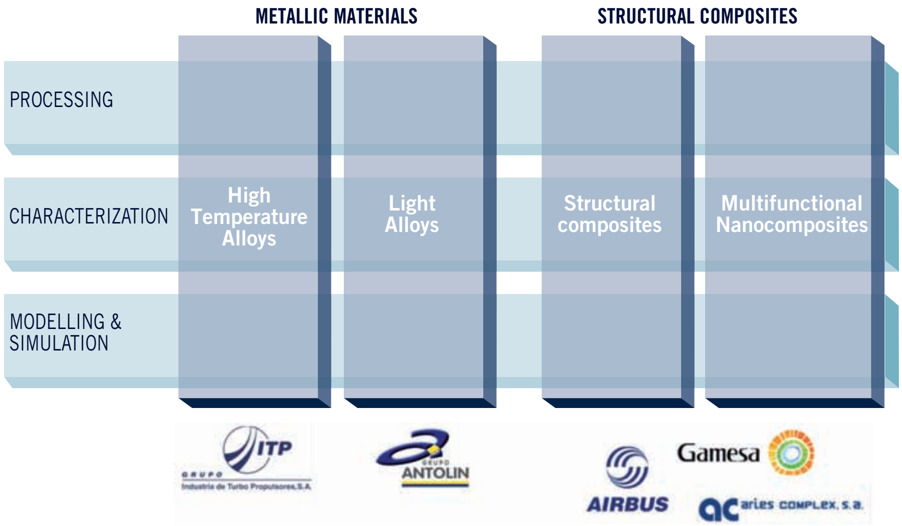


Figure 3. Vertical and horizontal research lines of IMDEA Materials.

2.1. Vertical Lines

Encompassing the research interests of the industrial partners, the vertical research lines of IMDEA Materials are directed towards processing, design and application of advanced structural materials in aerospace, automotive and energy generation sectors. Research activities are focalized in advanced metallic alloys and composites. The former are -and will be for a long time- the standard materials for structural applications in engineering, while the latter are the fastest growing class of structural materials.

Metallic Alloys

Metallic alloys have been studied for more than two hundred years and their processing, structure and properties are well established. Nevertheless, challenges in the areas of energy generation, transportation and health care are constantly demanding new metallic materials with improved properties (higher operation temperature, better strength/weight ratio), tailored behaviour or multifunctional capabilities (biocompatibility). The objectives of this research line include:

- Development of Ni/Co-based superalloys and intermetallic compounds to be used in high temperature structural applications in aggressive environments for long periods of time.
- Production of near net-shape components of advanced metallic alloys (W, Ni, Ti) from powders.
- Processing and characterization of thermal-barrier and antifriction coatings to improve the durability and structural integrity of critical components.
- Design of novel Mg alloys for die casting with improved mechanical properties, thermal conductivity and corrosion resistance.
- Processing and characterization of nanostructured metallic materials (Al, Zr, Mg, Ti, Ni, W) by severe plastic deformation to obtain new phases, novel microstructures with high strength and ductility and enhanced multifunctional capabilities (biocompatibility).

Composites

Composites are currently the best option for high-added value structural applications in aerospace, energy generation (wind turbines) and sports due to their outstanding properties in terms of specific stiffness and strength. Moreover, the dispersion of nanometric reinforcements can further enhance their mechanical properties and provide new functional capabilities, opening unexpected possibilities in many other applications (sensors, catalysis, water purification, health care). The objectives of this research line include:

- Development of thermoplastic composites for high temperature applications.
- Design of structural composites with high impact resistance.
- Development, characterization and simulation of multifunctional nanocomposites with improved mechanical properties and integrated functional capabilities (electrical conductivity, fire retardancy, UV and EMI shielding, biocide activity, etc.).
- Development of biodegradable and biocompatible structural composites and nanocomposites.

2.2. Horizontal Lines

Three horizontal areas of expertise have been identified, which cover the three remaining vertices of the Materials Science and Engineering tetrahedron: Processing, Characterization and Modelling. The techniques and expertise provided by these horizontal lines are readily applicable to any type of materials and processes, and support the research goals of the vertical lines. It should be noted that these horizontal activities are designed as actual research lines and also have their own research goals in the cutting edge of each area.

Processing

- Improvement of casting technologies (vacuum and inert atmosphere, equiaxed, directional and centrifugal) for Ni/Co-based superalloys and intermetallic compounds.
- Development of novel processing methods for metallic alloys based on rapid prototyping, electron-beam melting, direct-metal laser-sintering, spark-plasma sintering, severe plastic deformation, etc…
- Optimization of out-of-autoclave processing techniques for composites (pultrusion, RTM, SQ-RTM) to minimize defects and improve reliability.

Characterization

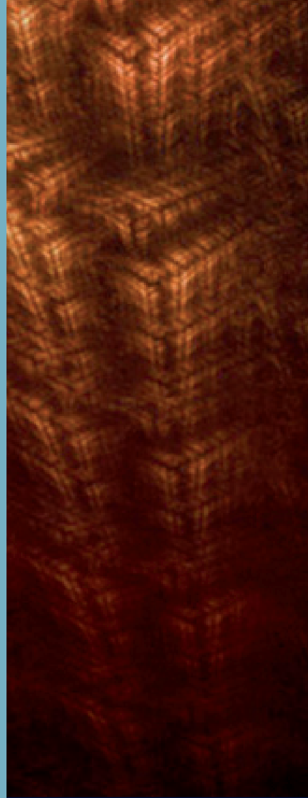
- Qualitative and quantitative characterization of the composition and microstructure of materials from the atomic level to the micron by means of different kinds of microscopy (approximation, scanning and transmission electron, optical, etc.), spectroscopy, X-ray diffraction and high-resolution three-dimensional computer assisted-tomography.
- Nano-mechanical and micro-mechanical characterization of the mechanical properties of materials at the nm and μm scale to establish the relationship between microstructure and properties.

Modelling and Simulation

- Development of multiscale modelling strategies to carry out virtual design and virtual processing (casting, forging, thermo-mechanical treatments) of metallic and composite materials (ab initio, molecular mechanics, computational thermodynamics, kinetic Monte Carlo, phase-field modelling, computational fluid dynamics, etc.).
- Development of multiscale modelling strategies to carry out virtual testing of metallic materials and composites (ab initio, molecular mechanics, dislocation dynamics, finite elements, homogenization, etc.).

3

research divisions



The research activities of IMDEA Materials are carried out in four research divisions devoted to Modelling & Simulation, Metallic Materials, Composites and Advanced Characterization.

3.1. Modelling & Simulation

This research division encompasses five research groups: Mechanics of Materials (Prof. J. LLorca), Theoretical and Applied Mechanics (Prof. P. Ponte-Castañeda), Computational Mechanics of Materials (Dr. A. Jérusalem), Multiscale Materials Modelling (Dr. J. Segurado) and Computational Materials Science (Dr. E. Martínez). Altogether, the expertise of the five research groups covers all the relevant simulation strategies to model the mechanical behaviour of materials from atomic scale to the dimensions of actual components, including ab initio, molecular mechanics, kinetic Monte Carlo, dislocation dynamics, finite elements and homogenization theory.

Research activities include the development of multiscale modelling tools to replace the costly certification tests required by the aerospace authorities by high fidelity numerical simulations. The research groups of Prof. LLorca and Dr. Segurado work in cooperation with Dr. González (Structural Composites) and Dr. Molina (Nanomechanics) to develop a novel virtual testing strategy. Starting from the in situ properties of fibre, matrix and interfaces, their efforts are directed to predict with accuracy the mechanical behaviour of individual lamina, laminates and small components using a cascade of simulation techniques based on computational micromechanics and mesomechanics. Current applications of this strategy are directed to analyze the effect of manufacturing defects in the performance of structural composites, to predict the behaviour of composite structures under hot/wet conditions and to assess the impact resistance of structural components for the next generation of Airbus aircrafts (A350XWB, A30X).

Homogenization is another multiscale simulation strategy to relate the microstructure with the macroscopic mechanical properties of thermoplastic elastomers and polycrystalline metals, pursued by the research groups of Prof. Ponte-Castañeda and Dr. Segurado, respectively. The emphasis of Prof. Ponte-Castañeda group is on the mathematical foundation of novel homogenization models which can take care of the strongly non-linear behaviour due to the materials' constitutive equation and to the microstructural evolution upon deformation. Dr. Segurado's efforts in this line are aimed at the implementation of the visco-plastic self-consistent approximation as a user material in commercial finite element codes. This is a significant step towards microstructurally-informed simulations of the mechanical behaviour of metallic components subjected to very large strains (deep drawing, impact, rolling, etc.).

Fundamental studies of size effects in the plastic deformation of FCC metals at the micron scale are carried out through the collaboration of the research groups of Dr. Martínez, Dr. Segurado and Prof. LLorca by means of dislocation dynamics simulations. In the field of atomistic modelling, Dr. Martinez's work is focused on the development of cohesive models based on ab initio density functional theory calculations to study the equilibrium phase diagrams of metallic alloys as well as the kinetics of phase transformations and radiation damage processes in these systems. At present, he is developing a simple concentration dependent model for Fe-Cr alloys, candidates for nuclear applications as structural materials, aimed at capturing all the rich thermodynamic and kinetic properties of the system. Modelling is based on Monte Carlo algorithms, an area in which he has developed a new parallel algorithm for the kinetic Monte Carlo which enhances its capabilities, being able to study larger systems during longer times.

The group of Dr. A Jérusalem, in tight collaboration with the Barcelona Supercomputing Center, is focused on very large scale parallel continuum simulations of material deformation. More specifically, the research activities involve the design and implementation of advanced algorithms for continuum simulations including parallel contact, fluid-solid interaction, or sophisticated techniques such as X-FEM. The materials studied range from traditional structural materials (composites and metallic alloys) to novel nanocrystalline metals, nanotwinned ultrafine crystals or individual biological cells.

3.2. Metallic Materials

The activities of IMDEA Materials in the area of Metallic Materials are distributed in four research groups devoted to Solid State Processing (Prof. J. M. Torralba), Metal Physics (Dr. M. T. Pérez-Prado), Computational Alloy Design (Dr. M. J. Santofimia) and Physical Simulation (Dr. I. Sabirov).

Prof. Torralba's group is working on the development of new metallic materials by powder technology techniques, as an alternative to conventional manufacturing routes, to improve properties and manufacture near-net shape components. Current activities are focused in a wide range of metallic materials including steels, light alloys (Ti and Mg), high temperature materials and metal matrix composites.

The Metal Physics and Physical Simulation groups, led by Dr. Pérez-Prado and Dr. Sabirov, respectively, approach metals innovation from a different perspective. The emphasis is placed on analyzing detailed microstructures processed by top-down techniques and relating parameters such as nature of the phases present, grain size and shape, texture, distribution of particles or density of dislocations, to the mechanical behaviour in a wide range of temperatures and strain rates.

Ultra-fine grained and nanostructured metals (Ti, Zr, Al-based) with enhanced properties have been processed using severe plastic deformation techniques (SPD) such as

equal channel angular pressing (ECAP), with or without parallel channels, high pressure torsion, accumulative roll bonding or sequential ECAP, swaging, and drawing. In particular, they have demonstrated that the combination of various processing techniques (ECAP, swaging, and drawing) is an effective tool for grain refinement down to ultrafine scale in a commercial pure Ti. Ultra-fine grained pure Ti presented an outstanding tensile strength of 1280 MPa and very anisotropic properties due to the strong texture created during the SPD processing. Current research activities are devoted to improve the ductility. High pressure torsion has also been used to induce phase transformations and to stabilize under ambient conditions, for the first time, high pressure phases of Zr whose properties are still unknown. This discovery has been patented and it is being applied to other transition metals.

Reducing CO_2 emissions and fuel consumption requires a significant reduction in the weight of automobiles and aerospace vehicles, and Dr. Pérez-Prado is also working in Mg alloys for structural applications. A significant effort is being placed in optimizing die-casting processes and in understanding the relationship among the microstructure, deformation micromechanisms (plastic slip, twinning) and mechanical behaviour at high strain rates and/or temperatures in a number of wrought and die cast Mg alloys (AZ31, AZ91, AM60).

In addition, the Physical Simulation group led by Dr. Sabirov will exploit the recently acquired Gleeble 3800 system to simulate industrial processes such as casting, welding, and forging as well as deformation processes in a fully controlled manner.

Finally, the research group of Dr. Santofimia focuses on the application of the quenching and partitioning process for the development of new class of low-carbon high strength steels. The chemical compositions of the steels were specially designed for this process, containing 3.5wt.% Mn to retard the formation of bainite and combinations of Si and Al to avoid cementite precipitation. A new kind of microstructure was generated, formed by laths of martensite separated by films of inter-critical ferrite and retained austenite. These new microstructures have led to improved properties of strength and ductility in comparison with current commercial high strength steels.

3.3. Composites

The activities of IMDEA Materials in the area of composites materials are performed by two research groups on Structural Composites and Multifunctional Nanocomposites led by Dr. González and Dr. Dasari, respectively. The activities of the Structural Composites group are focused in the optimization of out-of-autoclave processing techniques for aerospace applications. Current programs include the manufacturing of stiffeners and crossbars of C/epoxy composites with aerospace quality by pultrusion of carbon fabrics and

the development of same qualified resin transfer moulding (SQ-RTM) to manufacture structural composites by infiltration of pre-pegs. In addition, the group of Dr. González is working in close cooperation with the Divisions of Modelling & Simulation and of Advanced Characterization to manufacture composite panels with controlled defects for assessing the effects of defects in composites. Other areas of research include the development of new composite materials with enhanced impact resistance through the optimization of laminate sequence, the introduction of novel fabrics and the use of engineered interplies based on mats of electrospun nanofibres to achieve multi-functionality (mechanical, acoustic and conductive properties) in composite laminates.

The major research emphasis of Multi-functional Nanocomposites group is on the design, understanding and development of the next generation of eco-benign polymer nanocomposites for a wider range of applications. Current activities can be grouped into two broad areas: application of electrospinning technique and flame retardancy response of polymeric materials. In the first area, nanofibre mats made up of biodegradable and biocompatible polymers embedded with natural functional clays are manufactured by electrospinning as a novel alternate cost-effective wound dressing materials. The same technique is used to produce stable (physical/chemical), low cost, high flux, and anti-fouling organic-inorganic nanofibrous membranes for water treatment and purification processes. Finally, electrospun ZrO_2 nanofibres are used to enhance the biocompatibility of pure Zr implants. In the second area, the objective is to develop the next generation of 'green' polymer nanocomposites, which are environmentally friendly (halogen-free and phosphorus/phosphate-free) and exhibit superior thermal stability and excellent flame retardancy behaviour with balanced mechanical properties. Closely monitored activities include physical/chemical roles of nanoparticles, their migration and coupling, char enhancement, etc.

3.4. Advanced Characterization

This horizontal research line, led by Dr. J. Molina, is focused on advanced characterization techniques at the nm and µm level. In addition to standard techniques for microstructural characterization (TEM, SEM, X-ray diffraction, TGA, DSC, spectroscopy, etc.), a leading objective is to develop novel experimental methods to quantify mechanical properties at the nm and µm level. These include mechanical characterization of phases in heterogeneous materials, determination of size effects in the flow stress and strength of crystalline and amorphous materials, adhesion testing between dissimilar phases, assessment of local residual stresses which are caused by manufacturing processes as well as the determination of the deformation mechanisms. A close collaboration exists with the Division of Modelling & Simulation, as many of the current "complex" materials used for structural applications (nanostructured metals, multiphase alloys and/or composites) deform by unconventional mechanisms that need to be identified in order to develop physically-based models able to represent their mechanical behaviour.

Current techniques available include *in situ* mechanical testing within the scanning electron microscope, which offers the possibility to study the evolution of the microstructure upon loading, to map the strains in different phases using digital image correlation techniques and to capture the dynamics of deformation and fracture. In addition, Computer assisted X-ray microtomography is a powerful technique to visualize the 3D microstructure of materials up to the submicrometer range and to analyze the corresponding deformation and fracture micromechanisms. Finally, instrumented nanoidentation is used to extract critical material properties at the micro and nanoscale, including fibre/matrix interface and *in situ* matrix strength in composites, phase properties in polyphase metallic alloys, or in situations in which the amount of available material prevents the use of conventional mechanical tests.

4

scientists

IMDEA Materials is committed to attract talented researchers from around the world to work in Madrid in an international and interdisciplinary environment. Recruitment is carried out by means of International Calls for open positions, which are advertised in leading scientific journals and disseminated electronically throughout the scientific community. The initial international calls were launched in 2007 and 2008; 82 applications from scientists working in 18 different countries were received in 2007, while these numbers increased to 120 applications from 30 countries in 2008. Applications were reviewed by the members of the Scientific Council of IMDEA Materials, who selected 10 researchers in 2007 and 9 in 2008. Out of them, 5 senior researchers and 6 researchers (tenure-track) have joined IMDEA Materials. Their names and research areas are shown in Figure 4. In addition, IMDEA Materials team includes 4 post-doctoral research associates, 8 research assistants working towards their PhD and 1 technician. It should be noted that currently 39% of IMDEA researchers were born abroad. Another international call was recently opened to bring more talent in selected areas.

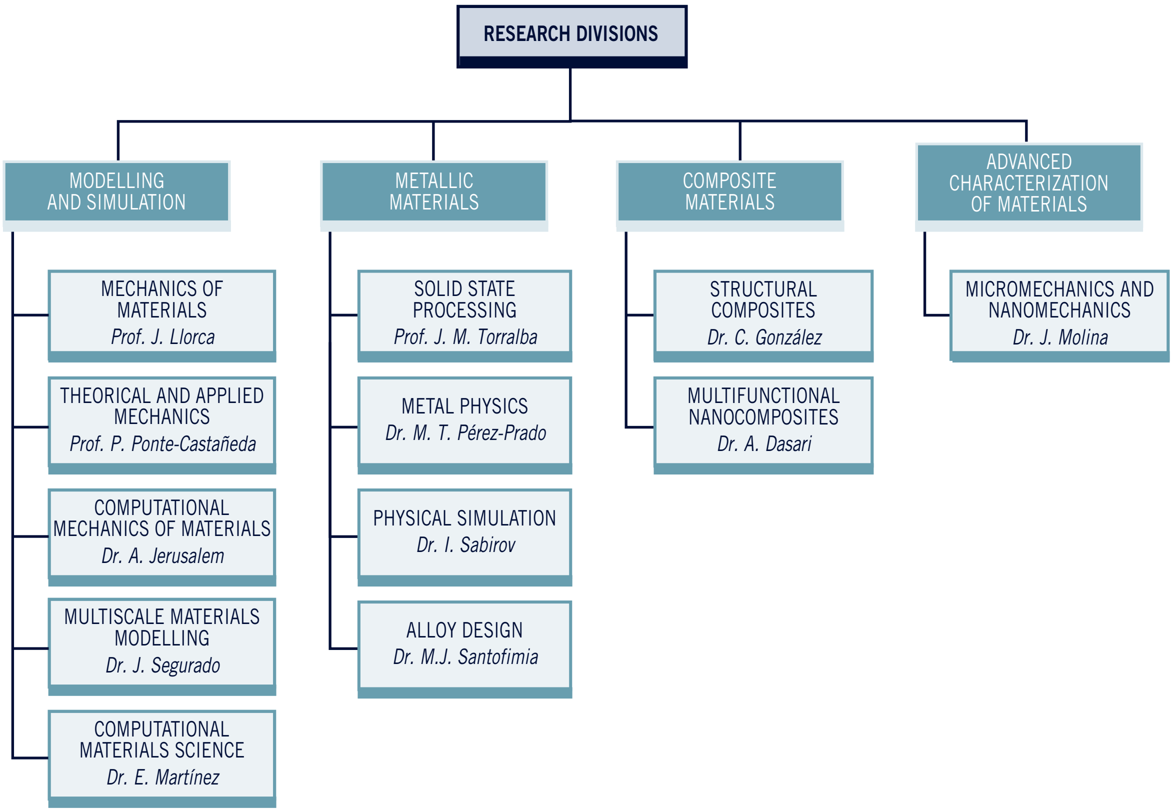
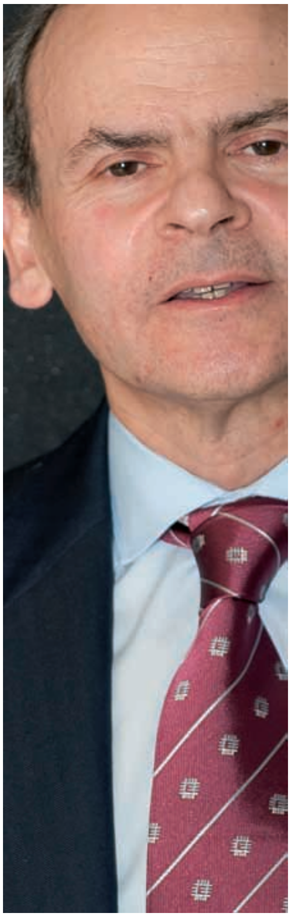


Figure 4. Researchers and research lines of IMDEA Materials.

scientists



Prof. Javier Llorca
Director
Mechanics of Materials

Javier LLorca graduated in Civil Engineering from the Polytechnic University of Madrid in 1983. He got his Ph. D. in Materials Science from the same institution in 1986. He leads the research group on "Advanced Structural Materials and Nanomaterials" at the Polytechnic University of Madrid and is Director of Madrid Institute for Advanced Studies of Materials (IMDEA Materials). Prof. LLorca has held positions as invited professor at Cornell (1986) and Brown University (1989-1990) and has received, among others, the Research Award of the Spanish Royal Academy of Sciences (1999), the Gold Medal from the Spanish Structural Integrity Society (2000) and the Research Award of the Polytechnic University of Madrid (2009). He has co-authored over 130 research papers in international peer-reviewed journals and has given about one hundred invited talks at national and international conferences and research centres throughout the world. He is member of the editorial board of Modelling and Simulation in Materials Science and Engineering, International Journal of Engineering Science and International Journal of Fatigue and Fracture of Engineering Materials and Structures. Prof. Llorca has participated in 40 research projects (25 as principal investigator) funded by national and international organizations and industries.

Research Interests
Prof. Llorca's research activity has been focused in the analysis of the relationship between microstructure and mechanical properties in advanced structural materials. In particular, he has developed novel multiscale simulation strategies to predict the macroscopic mechanical behaviour of materials from microstructural information as well as experimental characterization techniques to measure mechanical properties of materials under extreme conditions at microscopic and macroscopic levels. His contributions -particularly in the area of composite materials- have had a wide impact in the scientific community. Moreover, the advances in the areas of simulation and mechanical characterization have led to the development of new materials for structural applications, including polymer-, metal- and ceramic-matrix composites, nanocomposites, functionally-gradient materials, and eutectic ceramics.

Prof. José Manuel Torralba

Deputy Director

Solid State Processing

José Manuel Torralba graduated in Metallurgical Engineering in 1982 and obtained his Ph. D. in 1985 from the Polytechnic University of Madrid. He also got a degree in Armament and Material Engineering from the Army Polytechnic School in 1986. He is currently Professor of Materials Science and Engineering at the Carlos III University of Madrid, in which he has been Head of Department (1999-2000), Vice-rector for Academics Infrastructures (2000-2004) and Vice-rector for Research and Innovation (2004-2006). Since 2008, he is the Deputy Director of IMDEA Materials. He has co-authored over 130 papers in international peer-reviewed journal and has participated in 32 research projects funded by national and international organizations, 20 as principal investigator, and has been involved in several research grants funded by industry, including the Höganäs Chair in Powder Metallurgy. He has received several awards, including the "Professor Fryderyk Staub" from the Silesian University of Technology (2001), the Research Award of the Slovak Academy of Sciences (2005) and has received honorary degrees from the Technical University of Cluj-Napoca (2001) and the University of Craiova (2007). In the course of his tenure, he has advised 14 PhD theses and 35 MSc theses.

Research Interests

His main scientific-technical field of interest is the manufacturing of advanced structural materials by powder metallurgy, an area in which he has been working continuously since 1982. In this realm, he has made relevant contributions in the development of new alloying systems to improve sintering behaviour and structural properties of low-alloy steels, special steels (stainless and high speed steels) with improved corrosion and wear resistance, and metal-matrix composites, including different matrix materials as aluminum, iron or high speed steel. More recently, his research focus has broadened to include other processing technologies as mechanical alloying, metal injection moulding or spray pyrolysis to manufacture nanoparticles.

Prof. Pedro Ponte Castañeda

Associated Senior Researcher

Theoretical and Applied Mechanics

Pedro Ponte Castañeda was awarded a B.S. in Mechanical Engineering and a B.A. in Mathematics from Lehigh University in 1982. He received a M.S. in Engineering Sciences and a Ph.D. in Applied Mathematics from Harvard University in 1983 and 1986, respectively. Since 1990, he is a Professor and Graduate Group Chair in the Department of Mechanical Engineering and Applied Mechanics, and member of the Graduate Group in Applied Mathematics and Computational Science at the University of Pennsylvania. He has held visiting positions at the CNRS Laboratory of Mechanics and Acoustics in Marseilles (1993 and 2008), the Laboratory of Solid Mechanics at the Ecole Polytechnique in Paris (1994 and 2001) and the Department of Applied Mathematics and Theoretical Physics at Cambridge University (1994). He was elected to a Visiting Fellowship at Corpus Christi College (Cambridge) in 1994 and Professor of Mechanics at the Ecole Polytechnique in 2003. In 2009, Professor Ponte Castañeda joined IMDEA Materials as an associated senior researcher on a part-time basis. Professor Ponte Castañeda is currently Associate Editor of the Comptes Rendus Mécanique of the French Academy of Sciences, and of the Journal of Elasticity, as well as a member of the international advisory board of the Archives of Mechanics. He has published seminal papers in these fields and received in 2000 the Special Achievement Award for Young Investigators in Applied Mechanics from the American Society of Mechanical Engineers. In addition, he was the Midwest Mechanics Lecturer (2005-2006) and received in 2006 the George H. Heilmeier Faculty Award for Excellence in Research from the School of Engineering and Applied Science at the University of Pennsylvania.

Research Interests

Professor Ponte Castañeda's current research is concerned with the development of theoretical models for the physical and mechanical properties of heterogeneous material systems, specializing in nonlinear properties, microstructure evolution and applications to metal- and polymer-matrix composites, polycrystalline materials, active materials and geo-materials.

Dr. Carlos González

Senior Researcher

Structural Composites

Dr. Carlos González graduated in Civil Engineering in 1996 and obtained his Ph.D. in Materials Science in 2000 from the Polytechnic University of Madrid. Since 2007, he is an Associate Professor of Materials Science at this university. He currently leads the research group on Structural Composite at IMDEA Materials. Dr. González has published 30 papers in international peer-reviewed journals, several of which has been considered highly-cited papers by ISI and have been referenced in Science as seminal contributions in the topic of virtual simulations strategies. These research activities have been carried out within the framework of 15 research projects (4 as principal investigator) funded by regional, national and international organizations (particularly the European Union) and through contracts with leading national and multinational companies (Airbus, Rolls-Royce, Acciona, Anci, Future Fibers, etc).

Research Interests

His research activities have been focused in the characterization and modelling (theoretical and numerical) of the mechanical performance of advanced structural materials, with special emphasis in metal- and polymeric-matrix composites. Within this realm, the more significant contributions have been carried out to development of physically-based, micromechanical models of the deformation and fracture. These multiscale models are in the foundation of novel virtual testing strategies, which have opened revolutionary opportunities to reduce the number of costly tests to certify safety, to optimize materials configurations, to reduce development time (Right First Time), and to improve the accuracy of current phenomenological failure criteria.

Dr. Teresa Pérez Prado

Senior Researcher

Metal Physics

Teresa Pérez-Prado obtained her M.Sc. in Physics from the Complutense University of Madrid in 1994. After a brief stay at Chemnitz University, she joined the National Centre for Metals Research (CENIM, CSIC) in Madrid, where she worked in the superplastic deformation of aluminum alloys. She was awarded her Ph.D. in 1998 by the Complutense University of Madrid for this research, which was partially carried out at the Naval Postgraduate School in Monterey, California. From 1998 to 2001, Dr. Pérez Prado worked as a postdoctoral researcher at the University of California in San Diego and as a consultant at Oregon State University. She returned to CENIM in 2001 as a Ramón y Cajal fellow to work on the processing and physical metallurgy of novel Mg alloys for transportation. She was appointed Scientist in 2004, a position she held until 2008, when she joined IMDEA Materials as a Senior Researcher to lead the research group on Metal Physics. She has co-authored 1 book and over 55 papers in international peer-reviewed journals, and has held a visiting scientist position at the Max Planck Institute for Advanced Materials in Stuttgart in 2006. In addition, Dr. Pérez-Prado recently completed an MBA at Insead, France, where her team project, a spin-off company based on technology developed at Caltech and the University of Pittsburgh, was awarded the 1st prize at the Business Venture Competition.

Research Interests

Dr. Pérez-Prado´s current research interests involve applied and fundamental work on the processing, characterization and mechanical behaviour of advanced metallic materials for automotive, energy and biomedical applications.

Dr. Aravind Dasari

Researcher

Multifunctional Nanocomposites

Dr. A. Dasari graduated in Chemical Engineering from Jawaharlal Nehru Technological University (India) in 1999, and obtained a M.Sc. in Chemical Engineering from the University of Louisiana (USA) in 2003. He then moved to the University of Sydney (Australia) where he obtained his Ph.D. in 2007 from the Centre for Advanced Materials Technology (CAMT). During his PhD, he was awarded a highly competitive International Postgraduate Research Scholarship (IPRS) by the Australian Government and an International Postgraduate Award (IPA) by the University of Sydney. Upon completion of his PhD, he worked as a post-doctoral fellow at CAMT before becoming a Researcher at IMDEA Materials early 2009 to lead the research group on Multifunctional Nanocomposites. Dr Dasari has been invited to give plenary talks in several national/international conferences and workshops and was a Casual Lecturer at the University of Sydney from 2007-2008. Dr. Dasari was also a visiting scholar at Hong Kong University of Science and Technology in 2006. He has published 50 papers in peer-reviewed international journals, four book chapters, and many articles in conference proceedings. The quality of these contributions is also well reflected by h-index of 18. Recently, based on his research track record and standing in the field, he was included in the 10th Anniversary Edition (2008/2009) of 'Who's Who in Science and Engineering'.

Research Interests

Dr. Dasari has a general research interest on the processing-structure-property relationships of polymeric materials and more specifically, thermal stability/flame retardancy, tribology (at different length scales), and deformation/fracture mechanisms of polymer nanocomposites. He continues to work towards obtaining new generation of multi-functional and environmentally-friendly materials.

Dr. Antoine Jerusalem

Researcher

Computational Mechanics of Materials

Dr. Antoine Jérusalem graduated in 2004 with a double degree from the Ecole Nationale Supérieure de l'Aéronautique et de l'Espace with a Diplôme d'ingénieur, and from the Massachusetts Institute of Technology with a M.Sc. in Aeronautics and Astronautics. He obtained his Ph.D. in Computational Mechanics of Materials from MIT in 2007, where he stayed as a Postdoctoral Associate for an additional year. He became Researcher at IMDEA Materials in 2008, where he leads the research group on Computational Mechanics of Materials. Dr. Jérusalem has active collaborations in many different engineering and scientific fields with different institutes and universities around the world.

Research Interests

His research activities have focused on computational modelling of many types of materials and structures. Recently, he has been working on the modelling of nanocrystalline metals under loading rates ranging from quasi-static to shock, large-scale 3D parallel simulations of material fragmentation using Discontinuous Galerkin method, large-scale fluid-structure interaction simulations of the blast of human brain for traumatic brain injury studies as well as the modelling of deformation mechanisms of individual neurons.

Dr. Enrique Martínez

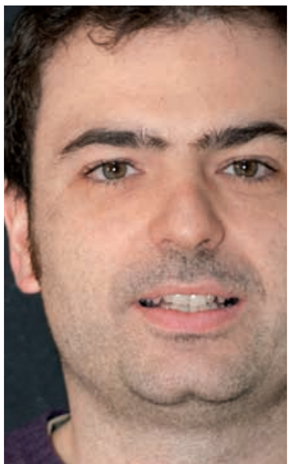
Researcher

Computational Materials Science

Dr. Enrique Martinez graduated in 2003 in Power Engineering from the Polytechnic University in Madrid and started his Ph.D. at the same University. In 2005 he was appointed as a researcher at the High Performance Computing Group, Lawrence Livermore National Laboratory in California, where he developed two advanced numerical algorithms, one for dealing with partial dislocations within a discrete dislocation dynamics methodology and the second to parallelize the kinetic Monte Carlo model via a synchronous strategy, which was able to extend the capabilities of such a model several orders of magnitude. After completing his Ph.D. work in 2008, Dr. Martínez obtained a postdoctoral position at the Commissariat à l'Énergie Atomique to work on the electronic properties of the Fe-Cr binary alloy and Fe-Cr-He ternary alloy. He obtained a Juan de la Cierva grant in 2009 and joined IMDEA Materials as Researcher and leader of the research group on Computational Materials Science.

Research Interests

His main scientific interests lay on the theoretical and computational multiscale modelling of materials. Particular emphasis is paid to the simulation of elastic and plastic processes using molecular dynamics and discrete dislocation dynamics methodologies, equilibrium thermodynamics and phase diagram calculations, non-equilibrium processes evaluated via Monte Carlo techniques and electronic structure of metallic alloys using density functional methods.



Dr. Jon Molina

Researcher

Micro- and Nano- Mechanics

Dr. Jon Molina-Aldereguía graduated in Materials Engineering from the University of Navarra in 1998 and got his Ph.D. from Cambridge University in 2002. Dr. Molina-Aldareguía held a postdoctoral position at the Department of Physics, University of Linköping (2003), and was Visiting Scientist at Intel Corporation during 2004. Afterwards, he got a tenured position at the CEIT and was appointed Associated Professor of Materials Science at the University of Navarre. He joined IMDEA Materials in 2008 as a Researcher and leader of the research group of Nanomechanics and Micromechanics of Advanced Materials. Dr. Molina has published more than 25 papers in international peer-reviewed journals, and this research was carried out within the framework of various research projects, both funded by industry and by national and European research programmes. Dr. Molina has participated in various Intel-sponsored projects to study the mechanical reliability of low-k interconnect structures for micro-processors (patterned thin-films), including the investigation of their cracking behaviour and the development of numerical models to predict their cohesive/adhesive failure. In addition, he is the coordinator of the European Project INTERFACE, funded by the European Union through the 6th Framework Program, which comprises 11 European institutions, to optimize the interface in carbon nanofibre reinforced Cu-matrix composites for thermal management applications.

Research Interests

His research interest lays on the broad subject of Micromechanics and Nanomechanics of multifunctional materials, and more specifically on the microstructural and mechanical characterization of thin-films, multiphase materials using nanoindentation and advanced focus-ion beam and electron microscopy analysis, including mechanical testing inside the scanning electron microscope.

Dr. Ilchat Sabirov

Researcher

Physical Simulation

Dr. Ilchat Sabirov obtained his Ms.C. in Materials Science and Engineering in 1999 from Ufa State Aviation Technical University (Ufa, Russia) and got his Ph.D. in Metallurgy from Montanuniversitaet Leoben (Leoben, Austria) in 2004. He held a postdoctoral position at the Erich Schmid Institute for Materials Science of the Austrian Academy of Science and later was appointed as an Academic Researcher at the Centre of Excellence for Design in Light Metals at Deakin University (Australia) in 2005. He also held visiting scholar positions at Technical University of Clausthal (2007) and at RWTH Aachen (2008) before joining IMDEA Materials in 2009 as a Researcher and leader of the research group of Physical Simulation of Metallic Materials. Dr. Sabirov has published 30 papers in international peer-reviewed journals and holds one international patent.

Research Interests

Dr. Sabirov's research interests focus on deformation processing of metallic materials, microstructure evolution during deformation processing, and physical simulation of these processes using state of the art GLEEBLE 3800 system. Particularly, he is interested in development of novel deformation processing routes for fabrication of advanced metallic materials with superior mechanical properties. Microstructure - deformation mechanisms - mechanical properties relationships are also of his interest. Another area of Dr. Sabirov's research is microstructure evolution during melting, solidification, and welding and the effect of processing parameters on local mechanical properties of superalloys.

Dr. Javier Segurado

Researcher

Multiscale Materials Modelling

Dr. Javier Segurado graduated in Materials Engineering from the Polytechnic University of Madrid in 1999 and got his Ph.D. from the same university in 2004. In 2008, he was appointed an Associate Professor at the Department of Materials Science, Polytechnic University of Madrid, and a Researcher at IMDEA Materials, where he leads the research group of Multiscale Modelling of Materials. Prior to these appointments, he held a position at the Institute of Light Weight Structures and Aerospace Engineering (Technical University of Vienna) and was a visiting scientist in the Materials Department, McMaster University (Ontario). Dr. Segurado is a co-author of 25 papers in international peer-reviewed journals, of which two have been considered highly-cited papers by ISI. This research has been carried out within the framework of 10 research projects (3 as principal investigator) funded by national and international research programs and industry.

Research Interests

His research interests are found in the broad area of multiscale modelling of structural materials and, within this realm, Dr. Segurado has worked on different materials and length scales. He has expertise in discrete dislocation dynamics and single-crystal plasticity models to study plastic deformation of metallic materials and in the development of computational micromechanics strategies to simulate the mechanical behaviour until failure of both particle and fibre reinforced composites.

Dr. María Jesús Santofimia

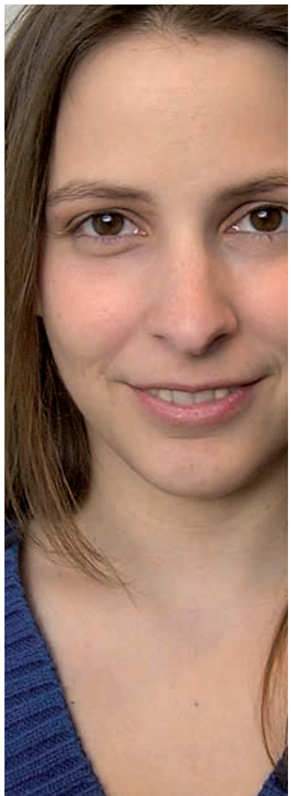
Researcher

Computational Alloy Design

Dr. Maria Jesus Santofimia graduated in Physics at the University of Cordoba in 2001. She carried out her Ph.D. work at the National Center for Metallurgical Research (CENIM-CSIC) and was awarded a Ph.D. in Physics of Materials by the Complutense University of Madrid in 2006. During this period, Dr. Santofimia held a short visiting scientist position at the Department of Materials Science and Metallurgy, University of Cambridge. Since 2006, Dr. Santofimia held a postdoctoral position in the Department of Materials Science and Engineering at the Delft University of Technology (The Netherlands). She got a Ramón y Cajal fellowship and joined IMDEA Materials in 2009 as a Researcher and leader of the research group on Computational Alloy Design. She has published 20 papers in international peer-reviewed journals and has been a principal researcher of a project for the development of high strength steels by the quenching and partitioning process.

Research Interests

The research interests of Dr. Santofimia are focused in the development of a new generation of high-strength, high-toughness steels for structural applications using novel thermo-mechanical treatments (quenching and partitioning method). The new alloys are designed using advanced computational thermodynamics tools to simulate the kinetics of phase transformations and the model predictions are verified through extensive mechanical and microstructural characterization of the materials.



postdoctoral research associates

Dr. Berta Herrero
Post-doctoral
Research Associate

Dr. Berta Herrero graduated in Chemistry in 1999 from the Autonomous University of Madrid and obtained an MsC in polymers from the Institute of Polymer Science and Technology (CSIC) and a Ph.D. in Chemistry from the Complutense University of Madrid in 2005. Afterwards, she worked for three years in Hutchinson, a multi-national company in the automotive sector, another year as an R&D consultant being responsible for the technical management of a FP7 European Project (FIRELI), and had visiting scholar appointment at the Institut für Makromoleculare Chemie of the Albert-Ludwigs University of Freiburg (Germany). Dr. Herrero joined the research group of Multifunctional Nanocomposites of IMDEA Materials as a postdoctoral Research Associate in 2009. She is a co-author of ten papers in international peer-reviewed journals and several technical reports for industry.

Her scientific interests are focused in processing and characterization of polymer nanocomposites for advanced applications. She has also expertise in fillers for rubber formulations, organically-modified nanoclays and flame retardant additives.

Dr. Rocío Seltzer
Post-doctoral
Research Associate

Dr. Rocío Seltzer graduated in Materials Engineering (2002) and obtained a Ms.C. in Materials Technology (2004) from the National University of Mar del Plata, Argentina. She obtained her Ph.D. degree in Materials Engineering at the Centre for Advanced Materials Technology of University of Sydney (Australia). Upon completion of her PhD, she worked as a research assistant at CAMT before assuming a Post-doctoral Research Associate Position in the Structural Composites group of IMDEA Materials in 2009. She has published seven papers in peer-reviewed international journals and has given several invited talks in national and international conferences and workshops.

Her research is currently focused on the optimization of out-of-autoclave processing techniques for advanced polymer composites and in the analysis of the structure/properties relationship of these materials by means of finite element simulations and advanced three-dimensional characterization techniques.

Dr. Federico Sket

Post-doctoral
Research Associate

Dr. Federico Sket graduated in Electrical Engineering from the National University of Comahue (Argentina) in 2005. Afterwards, he joined the Institute of Materials Science of Vienna University of Technology, where he carried out his diploma thesis on the characterization of corrosion resistance of functionally graded hardmetals. In 2006 he joined the Max-Planck Institute for Iron Research where he got his Ph.D. in 2009 through his work on X-ray tomography characterization of creep damage. He recently joined IMDEA Materials as a Postdoctoral Research Associate in the research group of Nanomechanics and Micromechanics. He has published seven papers in international peer-reviewed journals.

His research activity has been focused in the field of synchrotron computed tomography applied to creep and creep damage, using image analysis techniques, as well as in characterization of hardmetals produced by powder metallurgy techniques.

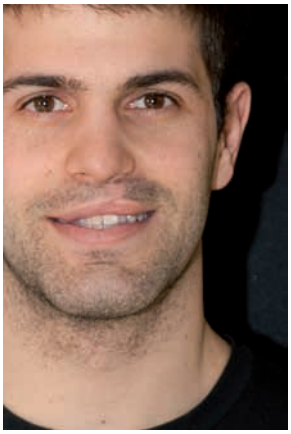
Dr. Katia Tamargo

Post-doctoral
Research Associate

Dr. Katia Tamargo-Martínez graduated in Chemistry from University of Oviedo in 1999 and obtained a Ph.D. in Chemistry in 2007 from the same institution for the work she carried out in the Chemistry of Materials Department at National Institute of Coal (CSIC). She joined IMDEA Materials in 2008 as a Postdoctoral Research Associate, where she is working in the micromechanisms of deformation and fracture of high-strength polymeric fibres.

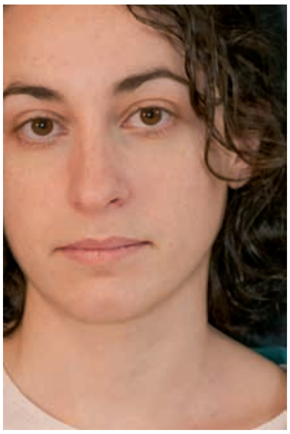
Her research expertise is focused in the properties of high-performance polymeric fibres (PBO, PPTA), with particular emphasis on the interfacial adhesion with epoxy matrices to improve the mechanical properties of composites. Within this area, she was worked on the surface modification of polymer fibres via plasma treatments, characterization of physical, chemical and mechanical properties of the modified fibres, and preparation and mechanical characterization of polymer-matrix composites.

predoctoral research assistants



Sergio Arias
MSc: Carlos III University of Madrid. Spain
Research: Micromechanics and nanomechanics

Nathamar Dudamell
MSc: Central University of Venezuela. Venezuela
Research: Physical metallurgy of Mg alloys



Silvia Hernández
MSc: Complutense University of Madrid. Spain
Research: Processing of composite materials

Eva Cristina Moreno
MSc: University of Castilla la Mancha, Spain
Research: Mechanical behaviour of nanostructured metals

Raúl Muñoz
MSc: Carlos III University of Madrid. Spain
Research: Computational mechanics of materials

Marcos Rodríguez
MSc: Complutense University of Madrid. Spain
Research: Micromechanics of composites

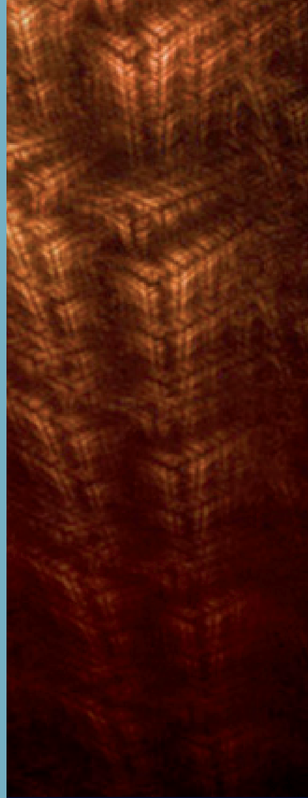
Sergio Sádaba
MSc: Public University of Navarre. Spain
Research: Virtual testing of composites

laboratory technician

Vanesa Martínez
MSc: University of Valencia. Spain

5

scientific infrastructures



IMDEA Materials' 2008-2011 strategic plan foresees an investment of approximately 7 M€ in research infrastructures in seven laboratories for processing of nanocomposites, processing of structural materials, chemical and microstructural characterization, nano- and micro-mechanics, mechanical characterization and computational materials science. Current facilities are located at the two provisional sites and include the following equipment:

5.1. Processing

- **Pultrusion Line** to manufacture continuous composite profiles of thermoset matrices reinforced with carbon, glass, aramid, and other advanced fibers. Fiber fabrics or roving are pulled off reels, guided through a resin bath or resin impregnation system and subsequently into a series of heated metallic dies to eliminate the excess of resin, obtain the correct shape and cure the resin. The pultruded continuous profile is extracted from the dies by means of hydraulic grips.

- **Resin Transfer Moulding** (Megaject MkV, Magnun Venus Plastech) to manufacture composite components with excellent surface finish, dimensional stability, and mechanical properties by low-pressure injection of thermoset polymers into a metallic mould containing the fibre preform.

- **Hot-Plate Press** (LabPro 400, Fontijne Presses) to consolidate laminate panels from pre-impregnated sheets of fibre-reinforced composites or nanocomposites by simultaneous application of pressure (up to 400 kN) and heat (up to 400ºC). Both thermoset and thermoplastic matrix composites can be processed.

- **Electrospinning Unit** (NANON-01A, MECC) to produce non-woven nanofibrous mats as well as aligned bundles of nanofibres based on various polymers, ceramics and composites. Nanofibres of different shape (smooth and porous surfaces, beaded, core-sheath) and orientations (non-woven cloth, aligned, and aligned multi-layer) can be manufactured.

- **Physical Simulation of Processing** (Gleeble 3800, DSI available in June 2010) to perform laboratory scale simulation of casting, welding, diffusion bonding and hot deformation processing (rolling, forging, extrusion) of a wide range of metallic alloys (steels, Ni-based superalloys, Ti, Al and Mg alloys, etc), as well as their thermo-mechanical characterization.

5.2. Microstructural and Mechanical Characterization

- **Scanning electron microscope** (EVO MA15, Zeiss) with automated pressure regulation from 10 to 400 Pa to work with non-metallic samples without the need of metalizing.

- **Micromechanical testing stages** (Kammrath and Weiss) to observe the specimen surface upon loading under light, scanning electron, focused ion-beam, scanning ultrasonic, or atomic force microscopy. Two stages prepared for tension/compression and fibre tensile testing are available, with maximum loads of 10 kN and 1 N, respectively.

- **Metallography laboratory** to prepare samples for microstructural analysis. Laboratory facilities include equipment for cutting, polishing and chemical etching, an optical microscope (Olympus BX-51) as well as an image analysis system for quantitative metallography.

- **X-ray computer-assisted 3D nanotomography scanner** (Nanotom, Phoenix) for three-dimensional visualization and quantitative analysis of microstructural features in a wide variety of materials ranging from metal powders and minerals to polymers and

biomaterials. The scanner combines a 160 KV X-ray source to study highly absorbing materials together with a nanofocus tube to provide high resolution (0.2-0.3 μm detail detectability).

- **Universal electromechanical testing machine** (Instron 3384) to characterize the mechanical properties of materials, include fixtures for different tests (tension, compression, bending, fracture), load cells (10 kN, 30 kN and 150 kN), and extensometers.

- **Rheometer** (AR2000EX, TA Instruments) to determine the rheological behaviour and viscoelastic properties of fluids, polymer melts, solids and reactive materials (resins) in the temperature range 25ºC to 400ºC.

5.3. Simulation

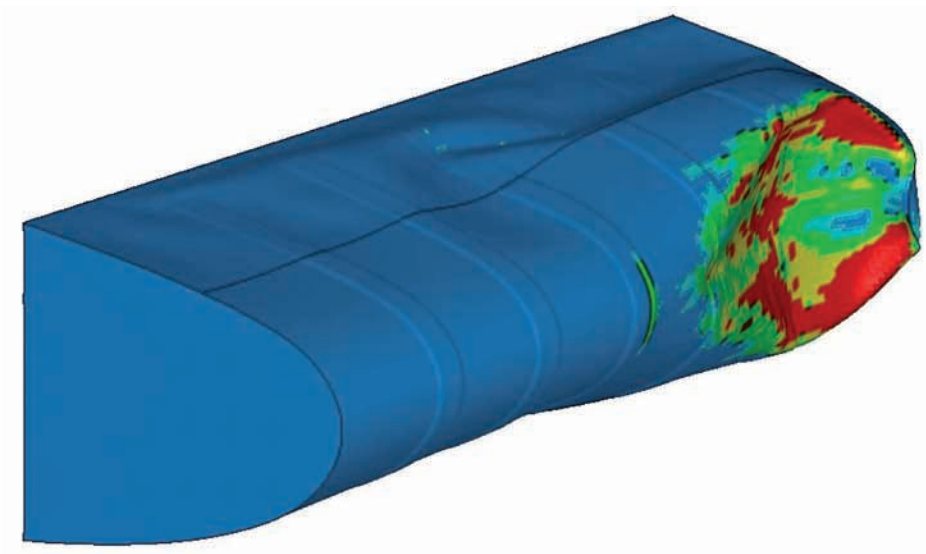
- **High performance computing cluster** (60 cores, AMD Opteron 2356 & 2431).

- **High performance computing servers** (8 cores AMD Opteron 8222SE, 8 cores INTEL Xeon X5450).

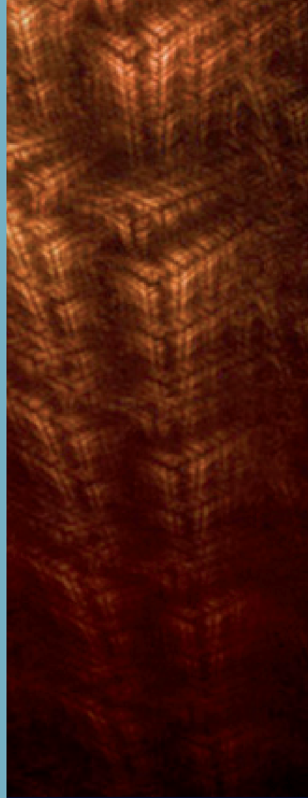
- Access to Mare Nostrum supercomputing facilities (Barcelona Supercomputing Center).

- Standard simulation, preprocessing and postprocessing packages (Abaqus, Hypermesh, Tecplot, etc.) as well as in-house developed codes for modelling and simulation of the mechanical behaviour and damage evolution of structural materials.

In addition to these research facilities, IMDEA Materials has signed collaborative agreements with universities and research institutions in Madrid to have access to singular research infrastructures which will not be available until the final site is completed.



6 research projects



Research activities and technology transfer to industry are normally carried out within the framework of research projects funded by national or international organizations or directly through contracts with industry. IMDEA Materials is already participating in a number of research projects in the areas of simulation, structural composites and nanocomposites, metallic materials and materials for electronics. A brief overview of the most relevant projects within each area is provided below:

MAAXIMUS

"More Affordable Aircraft Structure Lifecycle through eXtended, Integrated, & Mature nUmerical Sizing"

Funding: European Union, Transport-7th Framework Programme
Duration: 2008-2012
Principal Investigator: Prof. J. Llorca

MAAXIMUS is a collaborative research project funded by the European Union within the 7th Framework Program, in the topic "Integrated approach to life-cycle based development of aircraft structures." IMDEA Materials is one of the research centres in a consortium of 58 partners from 18 countries, coordinated by Airbus, made up of aircraft manufacturers, material behaviour specialists, software and computer hardware developers, computational mechanics experts and test centres, both from industry and the academic world. The budget for the project is approximately €70 M.

The project aims to reduce airframe development costs by 5% by delivering a predictive virtual test capability for large composite structures up to failure with a quantified level of confidence. This capability will be assessed and validated through an exhaustive comparison with a full-scale physical test of the composite barrel. A new Certification Philosophy, based on Virtual Testing, will be assessed. It will also consider the structure as it is actually manufactured and assembled, and not only as it is designed. Virtual Testing will be a major asset to freeze a trouble–free design earlier than today and will avoid last-minute and costly changes due to unexpected test results. It will also provide more mature aircraft to the customers at entry into service, with fewer service bulletins or post-entry-into-service modifications. This will be a key asset for airline satisfaction.

IMDEA Materials' contribution to the project will include the development of modelling tools to simulate the mechanical behaviour of composite materials and structures from microscopic to macroscopic level using computational micro- and mesomechanics, as well as the definition of a model to characterize composite material properties under hot/wet conditions.

FUTUREPBO

"Analysis and Optimization of PBO cables under service conditions")

Funding: Spanish Ministry of Science and Innovation (TRACE Programme 2008) and FUTURE FIBRES S.L.U.
Duration: 2008-2011
Principal Investigator: Dr. C. González

Due to their excellent mechanical properties, PBO poly (p-phenylene-2, 6-benzobisoxazole) fibres constitute one of today's most advanced polymeric fibres for structural applications. These fibres exhibit an outstanding specific stiffness and strength, and are very well suited for structural applications in which weight savings is critical.

Future Fibres is the world's leading designer, manufacturer and supplier of unidirectional PBO composite standing rigging for the high-performance yachting and super-yacht market. Future Fibres has a history of delivering innovative design, superior composite rigging solutions, unmatched technical experience and a proven track record – where weight savings and strength are critical. Many of the world's performance racing yachts entrust their composite rigging requirements to Future Fibres' exceptionally lightweight, incredibly strong and precisely engineered PBO composite rigging solutions.

In order to maintain its technological leadership, Future Fibres is working with IMDEA Materials in three critical areas: characterization of the behaviour of PBO under service conditions, characterization of PBO fibres failure micro-mechanisms, and development of analytical and numeric models to establish the relationship between the cable's internal structure and its mechanical behaviour under service conditions.

INTERFACE

Interfacial Engineering in Cu Carbon Nanofiber MMCs for high thermally loaded applications

Funding: European Union, NMP-6th Framework Programme
Duration: 2007-2009
Principal Investigator: Dr. J. M. Molina-Aldareguía

INTERFACE is a specific targeted research project funded by the European Union as part of the 6th Framework Program. IMDEA Materials is one of the research centres in a consortium of 11 partners from 8 countries, coordinated by CEIT (San Sebastian, Spain). The consortium is made up of experts in processing and modelling of nanocomposites materials, together with several end-users of heat sink devices in thermally high-loaded applications, such as high power laser diodes and electronics. The budget for this project is approximately €3 M.

INTERFACE's main objective is to gain the necessary knowledge to engineer the interface of Cu matrix composites reinforced by carbon nanofibres, to develop a low-cost material with a dramatically improved thermal conductivity. INTERFACE is driven by industry needs to develop more efficient low-cost heat sink materials for optoelectronics, LED displays, power switches and laser diodes, among others. The research will contribute to breakthroughs in the understanding of interfacial phenomena and to innovative means of fictionalization of carbon nanofibres, helping to develop a nanotechnology-based industry in Europe.

IMDEA Materials' contribution to the project includes the development of modelling tools to simulate the mechanical behaviour of nanocomposite materials from microscopic to macroscopic level using computational micro- and mesomechanics, as well as the thermo-mechanical characterization of interfaces.

MAGNO

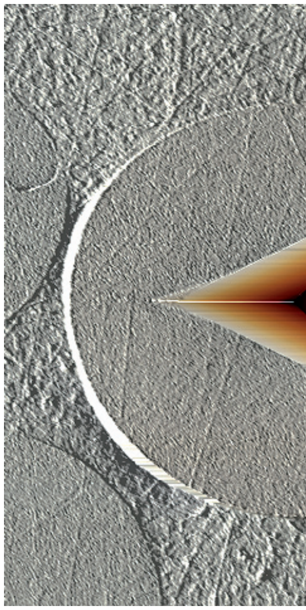
"MAGnesium New Technological Opportunities"

Funding: Spanish Ministry of Science and Innovation, CDTI (CENIT Programme)
Duration: 2008-2012
Principal Investigator: Dr. M.T. Pérez-Prado

MAGNO is a collaborative research project funded by the Centre for the Development of Industrial Technology (CDTI) as part of the fourth call of the National Strategic Consortiums of Technical Research (CENIT) program. With a total budget of €30 M, the MAGNO program is a national consortium comprising 12 companies and 11 technological centers under the guidance of the Grupo Antolín, a worldwide leader in the design and production of components and modules for cars.

The project is aimed at developing new technologies based on Magnesium alloys, an appealing material for structural applications in which weight reduction is a premium due to its low density. The automotive sector's shift towards more environmentally-friendly products using lighter components is driving the market to use Mg as a raw material to manufacture different parts. These developments are expected to spread to the aerospace and railway sectors as well.

IMDEA Materials' contribution to the project is focused on the development of new die cast Mg alloys with improved mechanical behaviour (yield strength, energy absorption by impact and creep resistance), corrosion resistance and higher thermal conductivity. This task also includes the fundamental understanding of the relationship between microstructure, deformation mechanisms and properties in traditional and novel Mg alloys, with particular emphasis in high strain rate and impact behaviour.



Other research projects of IMDEA Materials include:

IMS & CPS ("Innovative Material Synergies & Composite Processing Strategies")

Funding: European Union, NMP-7th Framework Programme
Partners: Coexpair (coordinator) and 15 more partners including EADS France and Alstom
Duration: 2010-2012
Principal Investigators: Dr. C. González and Dr. A. Dasari

ESTRUMAT ("Advanced Structural Materials")

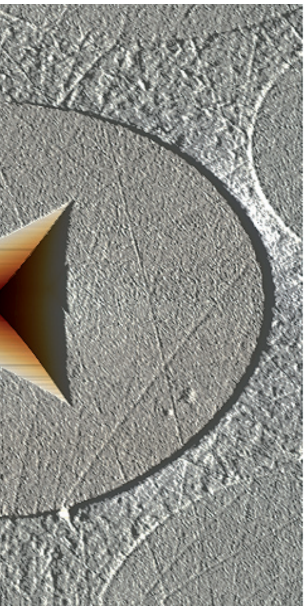
Funding: Regional Government of Madrid, General Direction for Research
Partners: Rey Juan Carlos University (coordinator), Polytechnic University of Madrid, Carlos III University of Madrid and Complutense University of Madrid
Duration: 2010-2013
Principal Investigator: Dr. M. T. Pérez-Prado

SINTONIA ("Innovative Material Synergies & Composite Processing Strategies")

Funding: Spanish Ministry of Science and Innovation, CDTI (CENIT Programme)
Partners: Coordinated by Boeing Research, collaboration with Aernnova Engineering
Duration: 2010-2012
Principal Investigator: Dr. J. Segurado

COMPOSIMPA ("Development of predictive numerical tools for the failure of composite structures under impact loadings")

Funding: European Union, 7th Framework Programme, ERA-Net SME
Partners: Principia (coordinator), Swerea-Sicomp and APC-Composite
Duration: 2010-2012
Principal Investigator: Dr. A. Jérusalem



ALTIVA ("Development of advanced gamma TiAl alloys for components with high reliability: microstructure design and modeling of the mechanical behavior")

Funding: Spanish Ministry of Science and Innovation (Fundamental Research Programme)
Partners: Carlos III University and Industria de Turbo Propulsores (ITP)
Duration: 2010-2012
Principal Investigator: Dr. M.T. Pérez-Prado

SIZEMATERS ("Size effects on the mechanical behavior of single crystals. Experiments and Simulations")

Funding: Spanish Ministry of Science and Innovation (Fundamental Research Programme)
Partners: Polytechnic University of Madrid
Duration: 2010-2012
Principal Investigator: Dr. J. M. Molina-Aldareguía

3D-CharMat ("3-Dimensional Characterization of Materials")

Funding: Spanish Ministry of Science and Innovation (Integrated Actions Programme)
Partners: Vienna University of Technology
Duration: 2010-2011
Principal Investigator: Dr. J. M. Molina-Aldareguía

FASENOVA ("New metallic materials by compression and shear")

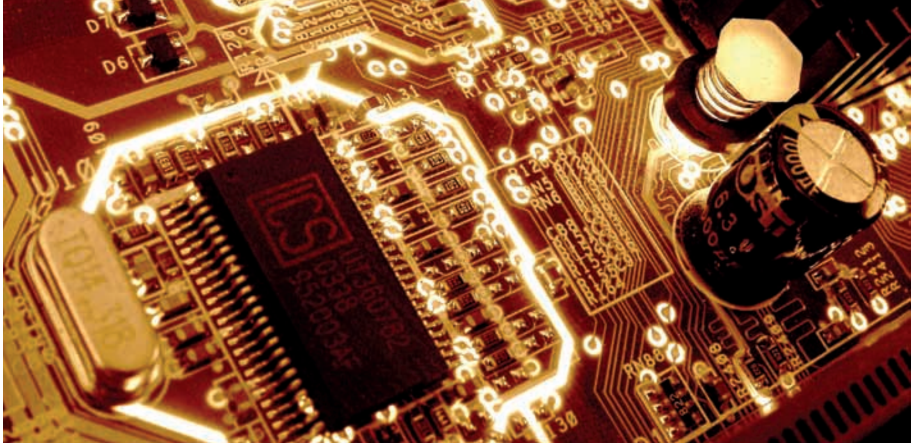
Funding: Spanish Ministry of Science and Innovation (EXPLORA Programme)
Duration: 2010-2011
Principal Investigator: Dr. M.T. Pérez-Prado

MORPHING ("Morphing materials for aeronautic applications")

Funding: Regional Government of Madrid, IMADE (PIE Programme)
Contractor: Aernnova Engineering Solutions Ibérica
Duration: 2009-2010
Principal Investigator: Dr. J. Segurado

DEFCOM ("The Effect of Defects in Structural Composites")

Funding: Europena Union, 6th Framework Programme, ERA-Net MATERA
Partners: Secar, Gamesa, Vienna University of Technology and Forschungs & Entwicklungs
Duration: 2009-2011
Principal Investigator: Prof. J. LLorca



ENGAGE ("Epitaxial Nanostructured GaAs on Si for Next Generation Electronics")

Funding: Europena Union, 6th Framework Programme, ERA-Net MATERA
Partners: Tyndall National Institute (coordinator), Dublin City University and the Institute of Materials Science of Madrid (CSIC)
Duration: 2009-2011
Principal Investigator: Dr. J. M. Molina-Aldareguía

ICARO ("Advance Composites Innovation and Rear end Optimization")

Funding: Spanish Ministry of Science and Innovation, CDTI (CENIT Programme)
Partners: Coordinate by Airbus, collaboration with Aries Complex and Airbus Military
Duration: 2009-2012
Principal Investigator: Dr. C. González

"Mechanical behaviour of aluminium alloys at high strain rates"

Contractor: Cenaero (Belgium)
Duration: 2008
Principal Investigator: Dr. J. Segurado

"Crack nucleation and propagation in Si buffers subjected to thermal loading"

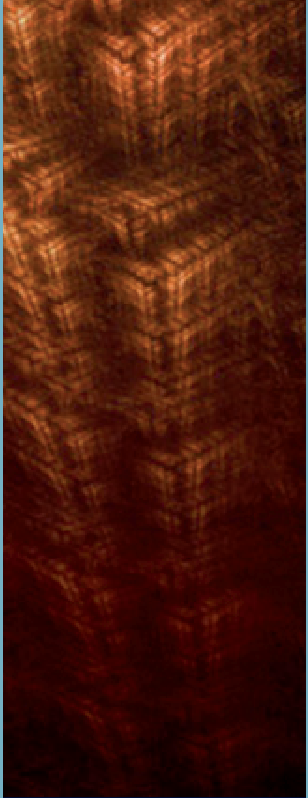
Contractor: Intel Ireland
Duration: 2008
Principal Investigator: Dr. J. Segurado

"Simulation of multiangular mechanical tests on prepreg composite coupons"

Contractor: Airbus Spain
Duration: 2007-2008
Principal Investigator: Prof. J. LLorca

"Simulations of the impact of a foreign object against a composite transmission shaft"

Contractor: Rolls-Royce
Duration: 2007-2008
Principal Investigator: Dr. C. González



7 dissemination results

publications 09

7.1. Publications

2009

1. I. Sabirov, M.R. Barnett, Y. Estrin, I. Timokhina, P.D. Hodgson. "*Deformation mechanisms in an ultra-fine grained Al alloy*". **International Journal of Materials Research 100**, 1679-1685, 2009

2. B.P. Kashyap, P.D. Hodgson, Y. Estrin, I. Timokhina, M.R. Barnett, I. Sabirov. "*Plastic flow properties and microstructural evolution in an ultra-fine grained Al-Mg-Si alloy at elevated temperatures*". **Metallurgical and Materials Transactions A 40**, 3294-3303, 2009

3. S. Malekjani, I.B. Timokhina, I. Sabirov, P.D. Hodgson. "*Deformation behavior of ultrafine grained steel produced by cold rolling of martensite*". **Canadian Metallurgical Quarterly 48**, 229-235, 2009

4. A. Dasari, Z.-Z. Yu, Y.-W. Mai. "*Electrically conductive and super-tough polyamide-based nanocomposites*". **Polymer 50**, 4112-4121, 2009

5. M.T. Pérez-Prado, A.P. Zhilyaev. "*First experimental observation of shear induced hcp to bcc transformation in pure Zr*". **Physical Review Letters 102**, 175504, 2009

6. B. Hutchinson, M.R. Barnett, A. Ghaderi, P. Cizek, I. Sabirov. "*Deformation modes and anisotropy in magnesium alloy AZ31*". **International Journal of Materials Research 100**, 556-563, 2009

7. A. Dasari, Z.-Z. Yu, Y.-W. Mai. "*Fundamental aspects and recent progress on wear/scratch damage in polymer nanocomposites*". **Materials Science and Engineering - Reports 63**, 31-80, 2009

8. A. Dasari, Z.-Z. Yu, Y.-W. Mai, G. Cai, H. Song. "*Roles of graphite oxide, clay and POSS during the combustion of polyamide 6*". **Polymer 50**, 1577-1585, 2009

9. A. Dasari, S.H. Lim, Z.-Z. Yu, Y.-W. Mai. "*Fracture properties and mechanisms of polyamide/clay nanocomposites*", in **"Nano- and Micromechanics of Polymer Blends and Composites"** (J. Karger-Kocsis, S. Fakirov, Eds.), Hanser, Munich, 377-423, 2009

10. M.R. Barnett, A. Ghaderi, I. Sabirov, B. Hutchinson. "*Role of grain boundary sliding in the anisotropy of magnesium alloys*". **Scripta Materialia 61**, 277-280, 2009

11. I. Sabirov, M.R. Barnett, Y. Estrin, P.D. Hodgson. "*The effect of strain rate on the deformation mechanisms and the strain rate sensitivity of an ultra-fine grained Al alloy*". **Scripta Materialia 61**, 181-184, 2009

12. E. Totry, C. González, J. LLorca, J. Molina-Aldareguía. "*Mechanisms of shear deformation in fiber-reinforced polymers: experiments and simulations*". **International Journal of Fracture 158**, 197-209, 2009

13. L. P. Canal, J. Segurado, J. LLorca. "*Failure surface of epoxy-modified fiber-reinforced composites under transverse tension and shear*". **International Journal of Solids and Structures 46**, 2265–2274, 2009

14. J. Moraleda, J. Segurado, J. Llorca. "*Effect of interface fracture on the tensile deformation of fiber-reinforced elastomers*". **International Journal of Solids and Structures 46**, 4287-4297, 2009

15. J. Moraleda, J. Segurado, J. LLorca. "*Finite deformation of incompressible fiber-reinforced elastomers: a computational micromechanics approach*". **Journal of the Mechanics and Physics of Solids 57**, 1596-1613, 2009

16. J. Segurado, J. LLorca. "*An analysis of the size effect on void growth in single crystals using discrete dislocation dynamics*". **Acta Materialia 57**, 1427-1436, 2009

17. M. V. Aguirre, A. Martín, J. Y. Pastor, J. Llorca, M. A. Monge, R. Pareja. "*Mechanical behavior of W-Y_2O_3 and W-Ti alloys from 25ºC to 1000ºC*". **Metallurgical and Materials Transactions A 40**, 2283-2290, 2009

18. D.F. Moore, A. Jérusalem, M. Nyein, L. Noels, M.S. Jaffee, R. Radovitzky. "*Computational biology - modeling of primary blast effects on the central nervous system*". **Neuroimage 47**, T10-T20, 2009

19. A. Jérusalem, R. Radovitzky. "*A continuum model of nanocrystalline metals under shock loading*". **Modelling and Simulation in Materials Science and Engineering 17**, 025001, 2009.

20. A. J. Clarke., J. G. Speer, D. K. Matlock, F. C. Rizzo, D. V. Edmonds, M. J. Santofimia. "*Influence of carbon partitioning kinetics on final austenite fraction during quenching and partitioning*". **Scripta Materialia 61**, 149-152, 2009

21. J. Marian, E. Martínez, H.J. Lee, B. Wirth. "*Micro/meso-scale computational study of dislocation-stacking-fault tetrahedron interactions in copper*". **Journal of Materials Research 24**, 3628-3635, 2009

22. N. Imaz, E. García-Lecina, C. Suarez, J. A. Díez, J. Rodríguez, J. Molina and V. García-Navas. "*Influence of additives and plating parameters on morphology and mechanical properties of copper coatings obtained by pulse electrodeposition*". **Transactions of the Institute of Metal Finishing 87**, 64-71, 2009

23. J.M. Córdoba, J. Tamayo-Ariztondo, J.M. Molina-Aldareguia, M.R. Elizalde and M. Odén. "*Morphology influence of the oxidation kinetics of carbon nanofibers*". **Corrosion Science 51**, 926-930, 2009

24. C.M. Moreno, J.M. Sánchez, L.C. Ardila and J.M. Molina-Aldareguía. "*Determination of residual stresses in cathodic arc coatings by means of the parallel beam glancing X-ray diffraction technique*". **Thin Solid Films 518**, 206-212, 2009

25. E. Ruiz-Hitzky, M. Darder, P. Aranda, M.A. Martín, G. del Real. "*Bionanocomposites as new carriers for influenza vaccines*". **Advanced Materials 21**, 4167-4171, 2009

26. V.J. Cadarso, A. Llobera, C. Fernández-Sánchez, M. Darder, C. Domínguez. "*Hollow waveguide-based full-field absorbance biosensor*". **Sensors and Actuators 139**, 143-149, 2009

publications 08

2008

1. E. Totry, C. González, J. LLorca. "*Prediction of the failure locus of C/PEEK composites under transverse compression and longitudinal shear through computational micromechanics*". **Composites Science and Technology 68**, 3128-3136, 2008

2. E. Totry, C. González, J. LLorca. "*Failure locus of fiber-reinforced composites under transverse compression and out-of-plane shear*". **Composites Science and Technology 68**, 829-839, 2008

3. E. Totry, C. González, J. LLorca. "*Influence of the loading path on the strength of fiber-reinforced composites subjected to transverse compression and shear*". **International Journal of Solids and Structures 45**, 1663-1675, 2008

4. T. E. Wilkes, J. Y. Pastor, J. Llorca, K. T. Faber. "*Mechanical properties of wood-derived silicon carbide Aluminum-Silicon-Magnesium composites as a function of temperature*". **Journal of Materials Research 23**, 1732-1743, 2008

5. T. E. Wilkes, J. Y. Pastor, J. LLorca, K. T. Faber. "*Mechanical properties of interpenetrating Al-SiC composites derived from wodd templates*". Proceedings of the **13th European Conference on Composite Materials**, electronic version, 2008

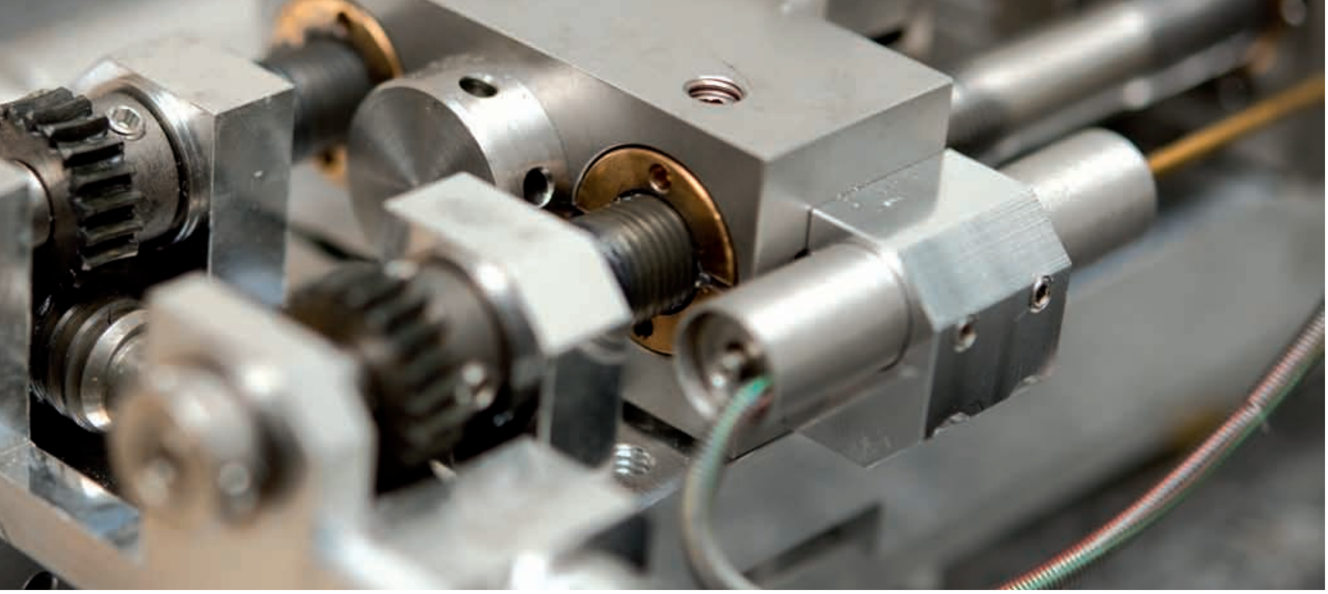
6. E. Totry, C. González, J. LLorca. "*Failure criteria for composite materials under multiaxial stress states*". Proceedings of the **13th European Conference on Composite Materials**, electronic version, 2008

7. A. Jérusalem, M. Dao, S. Suresh, R. Radovitzky. "*Three-dimensional model of strength and ductility of polycrystalline copper containing nanoscale twins*". **Acta Materialia 56**, 4647-4657, 2008

8. J. Neidhardt, C. Walter, J. M. Molina-Aldareguia, M. Herrmann, W. J. Clegg, L. Hultman. "*Transmission electron microscopy studies and simulation of the indentation response of superelastic fullerenelike carbon nitride thin films*". **Journal of Applied Physics 103**, 123515, 2008

9. I. Romero, J. Segurado, J. LLorca. "*Dislocation dynamics in non-conves domains using finite elements with embedded discontinuities*". **Modelling and Simulation In Materials Science and Engineering, 16**, 035008, 2008

10. E. M. Ruiz-Navas, M. L. Delgado, J. M. Torralba. *Aluminium PM: alloys and composites development and enhancement.* **Revista de Metalurgia 44**, 206-215, 2008.



11. M.I. Martin, M.E. Rabanal, L.S. Gómez, J.M. Torralba, O. Milosevic. "*Microstructural and morphological analysis of nanostructured alumina particles synthesized at low temperature via aerosol route*". **Journal of the European Ceramic Society 28**, 2487-2494, 2008

12. J.M. Contreras, A. Jiménez-Morales, J.M. Torralba. "*Improvement of rheological properties of inconel 718 MIM feedstock using tailored particle size distributions*". **Powder Metallurgy 51**, 103-106, 2008

13. M. Campos, J. M. Torralba, C. Menapace, A. Molinari. "*Effect of copper infiltration on fracture mode in sintered steels*". **Powder Metallurgy 51**, 176-181, 2008

14. M. Campos, L.Blanco, J. Sicre-Artalejo, J. M. Torralba. "*High performance low alloy steels: Up date*". **Revista de Metalurgia 44**, 5-12, 2008

15. J. Sicre-Artalejo, F. Petzoldt, M.Campos, J.M. Torralba. "*High-density inconel 718m: Three-dimensional printing coupled with hot isostatic pressing*". **International Journal of Powder Metallurgy 44**, 35-43, 2008

16. C.M. Tollan, R. Marcilla, J.A. Pomposo, J. Rodríguez, J. Aizpurua, J. Molina, D. Mecerreyes. "*Irreversible thermochromic behavior in gold and silver nanorod/polymeric ionic liquid nanocomposite films*". **Applied Materials and Interfaces 1**, 348-352, 2008

17. C.M. Moreno, J.M. Sánchez, J. Molina, F. Díaz and J. Fernández. "*Wear of chatodic arc coated WC-Co tools in the machinging of Ti-6Al-4V alloy*". **Int. J. Machining and Machinability of Materials 4**, 393-404, 2008

invited and plenary talks

7.2. International Congresses

Invited and Plenary Talks

1. *"Finite deformation of incompressible fiber-reinforced elastomers: a computational micromechanics approach"* J. Moraleda, J. Segurado and J. LLorca. **2009 Joint ASCE-ASME-SES Conference on Mechanics and Materials,** Blacksburg, Virginia, US, 2009

2. *"Superplastic deformation of Al_2O_3-$Y_3Al_5O_{12}$-YSZ eutectic ceramics"*. J. Y. Pastor, A. Martín, J. LLorca, P. B. Oliete, J. I. Peña, A. Larrea and V. M. Orera. **3th Directionally-Solidified Eutectic Ceramics Workshop,** Seville, Spain, 2009

3. *"Alpha to omega+beta transformation in pure Zr by high pressure torsion"*. M.T. Pérez-Prado and A.P. Zhilyaev. **International Conference on Processing & Manufacturing of Advanced Materials, Thermec'09 2009,** Berlin, Germany, 2009

4. *"From sintered iron to high performance PM steels"*. J.M. Torralba, R. De Oro, M. Campos. **RoPM'09. 4th International Conference on Powder Metallurgy,** Craiova, Romania, 2009

5. *"The complexity of the microstructural changes during the partitioning step of the quenching and partitioning process in low carbon steels"*. M. J. Santofimia, L. Zhao, Y. Takahama and J. Sietsma. **International Conference on Processing & Manufacturing of Advanced Materials, Thermec'09,** Berlin, Germany, 2009

6. *"Challenges in metal-nanofiber reinforced composites to obtain materials with high thermal conductivity"*. J.M. Molina-Aldareguía. **ASME 2nd Annual Multifunctional Nanocomposites and Nanomaterials (Euromed II Workshop),** Sharm El Sheikh, Egypt, January 11-13, 2008

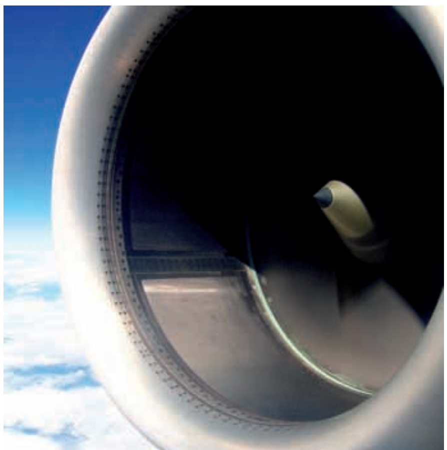
7. *"Multiscale modeling of structural composites: development of strategies for virtual testing"*. J. LLorca. **International Conference on Mathematics and Continuum Mechanics**, Oporto, Portugal, 2008

8. *"Void coalescence in model materials: experimental results and numerical simulations"*. J. LLorca, J. Segurado, A. Weck, D. S. Wilkinson and H. Böhm. **IUTAM Symposium on Theoretical, Modelling and Computational Aspects of Inelastic Media**. Cape Town, South Africa, 2008

9. *"Failure criteria for composite materials under multiaxial stress states"*. E. Totry, C. González and J. LLorca. **13th European Conference on Composite Materials**. Stockholm, Sweden, 2008

10. *"An experimental and numerical analysis of the V-notched rail shear test to measure the shear properties of fiber-reinforced polymers"*. E. Totry, C. González and J. LLorca. **4th International Conference on Composites Testing and Model Identification.** Dayton, Ohio, US, 2008

11. *"From sintered iron to high performance PM steels"*. J.M. Torralba, M. Campos. **X Congreso Iberoamericano de Metalurgia y Materiales,** Cartagena de Indias, Colombia, 2008



Regular Contributions

1. *"High strain rate behavior of Mg-Al alloys"*. N.V. Dudamell-Caballero, F. Gálvez and M.T. Pérez-Prado. **DFG– 8th International Conference on Magnesium Alloys and their Applications,** Weimar, Germany, 2009

2. *"Size and lattice orientation effects on ductile void growth in FCC single crystals"*. J. LLorca and J. Segurado. **2009 Joint ASCE-ASME-SES Conference on Mechanics and Materials,** Blacksburg, Virginia, US, 2009

3. *"Damage by decohesion during finite deformation of fiber-reinforced elastomers"*. J. Moraleda, J. Segurado and J. LLorca. **2009 Joint ASCE-ASME-SES Conference on Mechanics and Materials,** Blacksburg, Virginia, US, 2009

4. *"Failure micromechanisms & notch sensitivity of non-woven felts"*. A. Ridruejo, C. González and J. LLorca. **2009 Joint ASCE-ASME-SES Conference on Mechanics and Materials,** Blacksburg, Virginia, US, 2009

5. *"Role of nanoparticles on the ductility of HDPE"*. A. Dasari, Z.-Z. Yu and Y.-W. Mai. **The Fourth China-Europe Symposium on Processing and Properties of Reinforced Polymers,** Guilin, China, 2009

6. *"Discrete dislocation dynamics simulations of void growth in FCC single crystals"*. J. Segurado and J. LLorca. **10th US Congress on Computational Mechanics,** Columbus, Ohio, US, 2009

7. *"Simulation of void growth in FCC single crystals using discrete dislocation dynamics"*. J. Segurado and J. LLorca. **7th European Solid Mechanics Conference,** Lisbon, Portugal, 2009

8. *"Modelling Matrix Cracking in Fiber Reinforced Composites"*. S. Sádaba, C. González and J. Llorca. **V International Conference on Science and Technology of Composite Materials,** San Sebastián, Spain, 2009

9. *"Fracture mechanism of E-glass/epoxy composite laminates"*. E. Totry, J. Molina, C. González and J. Llorca. **V International Conference on Science and Technology of Composite Materials,** San Sebastián, Spain, 2009

10. *"Local effects on the fibre-matrix interfacial adhesion testing in fibre reinforced composites by the push-in/push-out test"*. J. Molina, M. Rodríguez, C. González and J. Llorca. **V International Conference on Science and Technology of Composite Materials,** San Sebastián, Spain, 2009

11. *"Extraction of matrix mechanical properties through in-situ nanoindentation testing of polymer matrix composites"*. M. Rodríguez, J.M. Molina-Aldareguía, C. González and J. Llorca. **17th International Conference on Composite Materials ICCM-17,** Edinburgh, UK, 2009

12. *"Failure analysis of impacted hybrid laminate composites using X ray tomography"*. A. Enfedaque, F. Gálvez, C. Gónzalez, J. Molina, G. Charalambous, J. Llorca. **V International Conference on Science and Technology of Composite Materials,** San Sebastián, Spain, 2009

13. *"Effects of Cr in He-vacancy clustering in dilute FeCr alloys from first principles"*. E. Martínez, C.C. Fu and F. Soisson. **14th International Conference on Fusion Reactors Materials,** Sapporo, Japan, 2009

14. *"Synchronous parallel kinetic Monte Carlo for discrete systems: The Ising model"*. E. Martínez, P. Monasterio, J. Marian and M.H. Kalos. **Materials Research Society Fall Meeting**, Boston, US, 2009

15. *"Structural variations and transcrystallinity in polymer nanocomposites"*. A. Dasari and Y.-W. Mai. **V International Conference on Science and Technology of Composite Materials,** San Sebastian, Spain, 2009

16. *"Effect of heat treatment of carbon nanofibres on copper deposition by electroless"*. J. Tamayo-Ariztondo, J.M. Córdoba, M. Odén, J.M. Molina-Aldareguía and M.R. Elizalde. **European Congress and Exhibition on Advanced Materials and Processes EUROMAT 2009,** Glasgow, UK, 2009

17. *"Predicting the thermal conductivity of composite materials with anisotropic inclusions and an imperfect interface"*. D. Marcos-Gómez, J. Ching-Lloyd, M. R. Elizalde, W. J. Clegg, J. M. Molina-Aldareguía. **European Congress and Exhibition on Advanced Materials and Processes EUROMAT 2009,** Glasgow, UK, 2009

18. *"Thermomechanical properties of copper-carbon nanofibres composites prepared by spark plasma sintering and hot pressing"*. J. M. Ullbrand, J. M. Córdoba, J. Tamayo-Ariztondo, M. R. Elizalde, M. Nygren, J. M. Molina-Aldareguía and M. Odén. **European Congress and Exhibition on Advanced Materials and Processes EUROMAT 2009,** Glasgow, UK, 2009

19. *"Fibre-Matrix interfacial strength measurement using the push-in test. Nanomechanical testing"*. J.M. Molina-Aldareguía, M. Rodríguez, C. González and J. Llorca. *Local Effects on the* **Nanomechanical Testing in Materials Research and Development,** Barga, Italy, 2009

20. *"Processing of ball-milled Fe-Mn master alloy powder: description of the formation"*. J. Sicre-Artalejo, M. Campos, J.M. Torralba. **EURO PM'09,** Copenhague, Denmark, 2009

21. *"Analytical determination of critical crack sizes in Si wafers"*. J.M. Molina-Aldareguía, J. Segurado. **Intel European Research and Innovation Conference 2008,** Dublin, Irland, 2008

22. *"Comprehensive characterization of mechanical properties of heat-treated low-alloyed steels with Mn added via mechanical alloying"*. M. Campos, José A. Sicre-Artalejo, J.M. Molina-Aldareguía and José M. Torralba. **2008 World Congress on Powder Metallurgy & Particulate Materials,** Washington D.C., US, 2008

23. *"Failure surface of a rubber-modified epoxy C-fiber composite under multiaxial loading"*. L. P. Canal, J. Segurado and J. LLorca. **45th Annual Meeting of the Society of Engineering Science,** Urbana- Champaign, Illinois, US, 2008

24. *"Analysis of the size effect in void growth in single crystals using discrete dislocation dynamics"*. J. Segurado and J. Llorca. **45th Annual Meeting of the Society of Engineering Science,** Urbana- Champaign, Illinois, US**,** 2008

25. *"Virtual testing of composite laminate coupons"*. C. González, J. Llorca and S. Sádaba. **8th. World Congress on Computational Mechanics (WCCM8),** Venice, Italy, 2008

26. *"An analysis of damage accumulation in composite materials using computational micromechanics".* S. Sádaba, C. González and J. LLorca. **8th World Congress on Computational Mechanics (WCCM8),** Venice, Italy, 2008

27. *"Three-dimensional model of nanotwinned ultrafine crystalline copper".* A. Jérusalem, M. Dao, S. Suresh and R. Radovitzky. ***ASME International Mechanical Engineering Congress and Exposition,*** Boston**,** MA, US, 2008

28. *"Modeling blast-related traumatic brain injury".* M. Nyein, A. Jérusalem and R. Radovitzky. **ASME International Mechanical Engineering Congress and Exposition,** Boston, MA, US, 2008

29. *"Modeling blast-related brain injury".* M. Nyein, A. Jérusalem, R. Radovitzky, D. Moore, L. Noels. ***26th Army Science Conference,*** Orlando, FL, US, 2008

30. *"Modeling blast-related traumatic brain injury".* M. Nyein, A. Jérusalem and R. Radovitzky. **8th World Congress on Computational Mechanics,** Venice, Italy, 2008

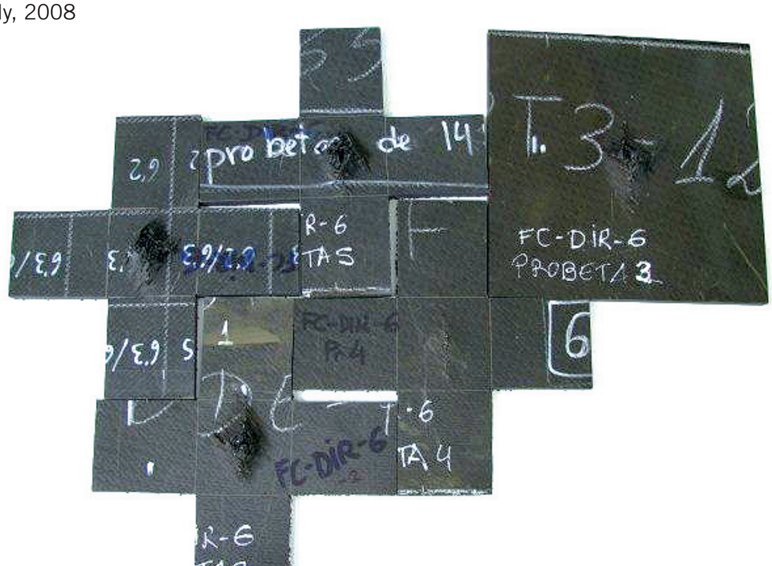
31. *"Three-dimensional massively parallel simulation of dynamic fracture and fragmentation using a hybrid DG/Cohesive method".* A. Seagraves, A. Jérusalem, L. Noels and R. Radovitzky. **8th World Congress on Computational Mechanics,** Venice, Italy, 2008

32. *"Three-dimensional model of nanotwinned ultrafine crystalline copper".* A. Jérusalem, M. Dao, R. Radovitzky and S. Suresh. **8th World Congress on Computational Mechanics**, Venice, Italy, 2008

33. *"Comparative behavior of bronze and superalloy feedstocks made with different particle sizes".* J.M. Contreras, A. Jiménez-Morales, J.M. Torralba. **2008 World Congress on Powder Metallurgy & Particulate Materials,** Washington, US, 2008

34. *"Development of diffusion-alloyed powders using Cu-Ni diffusion-alloyed particles on Fe and Fe-Mo base materials".* F. Cortés, A. Viejo, J. Sicre-Artalejo, M. Campos, J.M. Torralba, D.R. Amador. **2008 World Congress on Powder Metallurgy for Automotive Parts,** Isfahan, Iran, 2008

35. *"Comprehensive characterization of mechanical properties of heat-treated low alloyed steels with Mn added via mechanical alloying".* J. Sicre-Artalejo, M. Campos, J.M. Torralba. **2008 Powder Metallurgy World Congress & Exhibition,** Washington, US, 2008



7.3. Invited Seminars and Lectures

1. *"Materials and life"*. M.T. Pérez-Prado. IX Jornada de Materiales. **Carlos III University of Madrid,** Leganés, Spain, 2009

2. *"Bulk nanostructured hcp metals by severe plastic deformation"*. M.T. Pérez-Prado. MagIC - **Magnesium Innovation Centre, GKSS Research Center,** Geesthacht, Germany, 2009

3. *"Virtual testing of composites: an application of multiscale modelling of materials"*. J. LLorca. Institute des Matériaux. **Ecole Polytechnique Fédérale de Lausanne**, Switzerland, 2009

4. *"Modelling deformation and fracture of engineering materials at the micron scale"*. J. LLorca. Centre des Materiaux, **Ecole des Mines,** Evry, France, 2009

5. *"Modelling ductile fracture at the micron scale"*. J. LLorca. Department of Mechanical Engineering, **Columbia University**, New York, US, 2009

6. *"Towards multi-functional polymer nanocomposites"*. A. Dasari. College of Materials Science and Engineering, **Beijing University of Chemical Technology**, China, 2009

7. *"Materials in microelectronics"*. J. Molina. XI Workshop of Materials: The materials in the centre of our engineering activity. Escuela Politécnica Superior, **Carlos III University of Madrid,** Leganés, Spain, 2009

8. *"Void growth inside single crystals using discrete dislocation dynamics"*. J. Segurado. **Los Alamos National Laboratory**, New Mexico, US, 2009

9. *"Void growth inside single crystals using discrete dislocation dynamics"*. J. Segurado. **Lawrence Livermore National Laboratory**, California, US, 2009

10. *"What is powder metallurgy"*. J.M. Torralba. **European Powder Metallurgy Association (EPMA)** Summer School, Kosice, Slovak Republic, 2009

11. *"Powder metallurgy ligth alloys"*. J.M. Torralba. **European Powder Metallurgy Association (EPMA)** Summer School, Kosice, Slovak Republic, 2009

12. *"Porous materials"*. J.M. Torralba. **European Powder Metallurgy Association (EPMA)** Summer School, Kosice, Slovak Republic, 2009

13. *"Multidisciplinary applications in computational mechanics"*. A. Jerusalem. **Polytechnic University of Madrid**, Spain, 2008

14. *"Hexagonal nanomaterials processing via severe deformation"*. M.T. Pérez-Prado. **Polytechnic University of Madrid**, Spain, 2008

15. *"Modelling deformation and fracture of engineering materials at the micron scale"*. J. LLorca. **Erich Schmid Institute of Materials Sciences, Austrian Academy of Sciences,** Leoben, Austria, 2008

16. *"Virtual testing of Composites: from materials to components*". J. LLorca. Department of Aeronautics and Astronautics. **Purdue University.** West Lafayette, Indiana, US, 2008

17. *"Virtual testing of composites: from materials to components"*. J. LLorca. Department of Aerospace Enginnering and Engineering Mechanics. **University of Texas at Austin**, Texas, US, 2008

18. *"Virtual testing of composites: from materials to components"*. J. Llorca. Department of Aerospace Engineering. **Texas A&M University,** College Station, Texas, US, 2008

19. *"Virtual testing of composites: an application of multiscale modelling of materials"*. J. Llorca. **Technology Convention of ITP,** Madrid, Spain, 2008

20. *"Discrete dislocation dynamics: a powerful strategy to study size effects in crystalline materials at the micron scale"*. J. LLorca. **NANOMEC Network,** Madrid, Spain, 2008

21. *"Virtual testing of composites: from materials to components"*. J. LLorca. Summer Course on Composites Materials, **Polytechnic University of Madrid**, Spain, 2008

7.4. Organization of Conferences, Workshops and Courses

1. Symposium B17-Metal Matrix Composites Reinforced with Nano-sized Reinforcements. European Congress and Exhibition on Advanced Materials and Processes EUROMAT. J.M. Molina-Aldareguía. Glasgow, UK, 2009

2. 3rd International Directionally-Solidified Eutectics Workshop. J. LLorca. Seville, Spain, 2009

3. European Powder Metallurgy Congress. J.M. Torralba. Copenhaven, Dennmark, 2009

4. VII Internatinal Latin American Conference on Powder Technolgy. J.M. Torralba. Atibaia, Sao Paulo, Brazil, 2009

5. AMME'08 Achievements in Mechanical and Materials Engineering. J.M. Torralba. Gliwice-Ryn, Poland, 2009

6. European Powder Metallurgy Association (EPMA) Summer School. J.M. Torralba. Kosice, Slovak Republic, 2009

7. IACM-IUTAM International Symposium on Virtual Testing of Composite Materials and Structures, 8th World Congress on Computational Mechanics. J. LLorca. Venice, Italy, 2008

8. II National Congress of Powder Metallurgy. J.M. Torralba. San Sebastián, Spain, 2008

9. Homogenization-based Polycrystal Plasticity Models Course. R. Lebensohn. IMDEA Materials, Madrid, Spain, 2008

conferences
workshops
courses

seminars

7.5. Seminars

"Structure-property relationships for die-cast AM60B magnesium alloy". **J.P. Weiler** (from University of Western Ontario), 2009

"Manufacturing aspects of thermoplastic composites and special development of nanomodified polymers for tribology applications". **K. Friedrich** (from Institute for Composite Materials and Technical University of Kaiserslautern), 2009

"Titanium metal matrix composites reinforced with Boron and Carbon base reinforcements by Powder Metallurgy technology". **I. Montealegre** (from Austrian Research Centers GmbH-ARC), 2009

"The influence of alloying elements and process parameters on the mechanical properties of magnesium sheets". **D. Leyzig** (from GKSS Institute), 2009

"The influence of alloying elements and extrusion parameters on the room temperature mechanical properties of extruded magnesium alloys". **J. Bohlen** (from GKSS Institute), 2009

"Physical metallurgy of phase transformations in solid-state metals". **J. Sietsma** (from Delft University of Technology), 2009

"Simulation of damage evolution in composites: a phase-field model". **B. Biner** (from Ames Laboratory, Iowa State University), 2009

"Mechanical behavior of cast Mg alloys". **M. Aljarrah** (from University of Western Ontario), 2009

"A scalable discontinuous Galerkin method for brittle fracture". **R. Radovitzky** (from Massachusetts Institute of Technology), 2009

"Using high-pressure torsion for metal processing: fundamentals and applications". **A. P. Zhilyaev** (from National Center for Metallurgical Research, CSIC and Institute for Metals Superplasticity Problems, Ufa, Russia), 2008

"Atomic-level computer modeling of FeCr alloys for nuclear applications". **L. Malerba** (from Studiecentrum voor kernenergie, Centre d'études de l'énergie nucléaire. Belgium), 2008

"Specimen size effects on tensile strength and failure mechanisms of carbon/epoxy composites". **M.R. Wisnom** (from University of Bristol), 2008

"Mesostructured forms of transition alumina". **T.J. Pinnavaia** (from Michigan State University), 2008

"Macroscopic behavior and field statistics in viscoplastic composites". **M.I. Idiart** (from Cambridge University), 2008

"Continuum finite element simulations of sharp indentation experiments across the material length scales". **J. Alcalá** (from Polytechnic University of Catalonia)

"Simulation of Defect Evolution in Irradiated Materials: Kinetic Monte Carlo vs Rate Theory". **C.J. Ortiz** (from CIEMAT), 2009

"Size effects and strain gradient plasticity: how many Length scales should be involved in the modelling". **L. Bardella** (from University of Brescia), 2009

"Scale transitions in the plasticity of F.C.C. single crystals". **L. Kubin** (from Onera, France), 2009

"Twinning stress determination from first principles". **H. Sehitoglu** (from University of Illinois at Urbana-Champaign), 2009

"Onset of cavitation in hyperelastic solids under arbitrary loading conditions". **O. López-Pamiés** (from State University of New York), 2009

7.6. Fellowships

Marie Curie AMAROUT Incoming Fellowships, European Union-7th Framework Programme, 2009. (**Dr. R. Seltzer, Dr. A. Dasari and Dr I. Sabirov**)

Incentive for the Incorporation and Intensification of Research Activity (I3) Fellowships, Spanish Ministry of Science and Innovation, 2009. (**Dr. M.T. Pérez-Prado and Dr. J.M. Molina Aldareguía**)

Ramon y Cajal Fellowships, Spanish Ministry of Science and Innovation. 2009 (**Dr. M.J. Santofimia**) and 2008 (**Dr. M. Darder**)

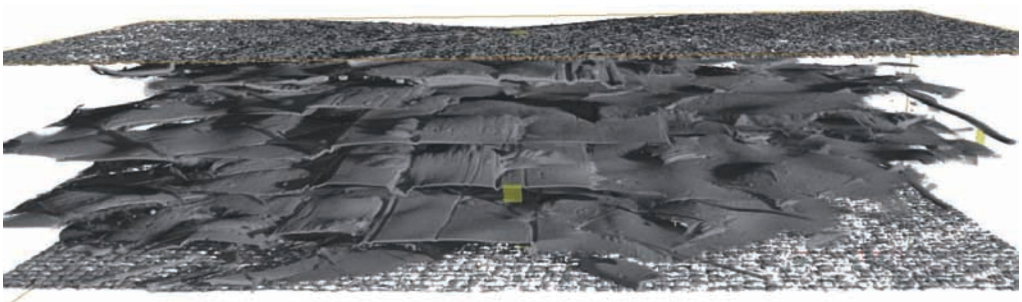
Juan de la Cierva Fellowships, Spanish Ministry of Science and Innovation, 2009 (**Dr. A. Jerusalem** and **Dr. E. Martínez**)

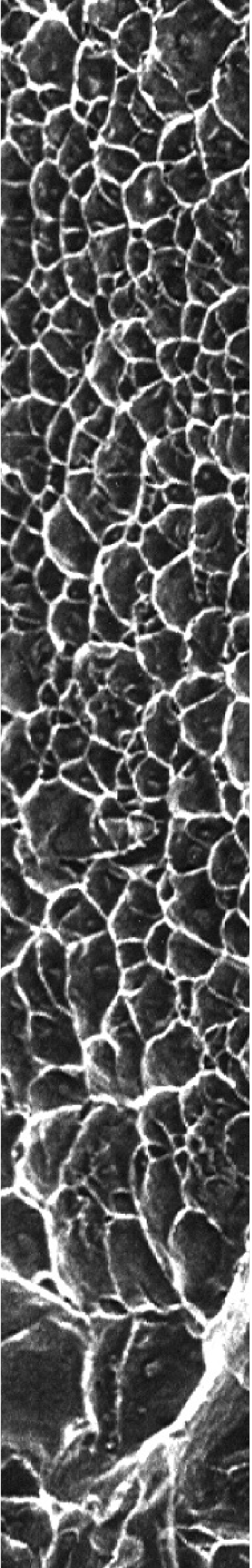
7.7. Awards

- **Prof. J. Llorca**. Research Award of the Polytechnic University of Madrid (2009)
- **Dr. E. Martínez**. *Award to the best doctoral thesis, Polytechnic University of Madrid* (2009)
- **Prof. J. Llorca**. Elected to the Royal Academy of Sciences of Zaragoza (2008)

7.8. Institutional Activities

- Member of the Steering Committee of the *Spanish Technological Platform of Advanced Materials and Nanomaterials* (MATERPLAT)
- Member of the Technological Clusters on Security and Renewable Energies promoted by *Instituto Madrileño para el Desarrollo* (IMADE)
- Incorporation to the Network of Research Laboratories of *Comunidad de Madrid* (REDLAB)
- Collaboration with the Department of Materials Science, Polytechnic University of Madrid to organize the *Materials Science Frontiers* Seminars
- Coorganizers of the Interuniversity Research Seminars Programme (R. Ogden, R. Abeyaratne, A. Needleman and D. Leguillon)
- Participation in the *"VIII and IX Semana de la Ciencia",* Madrid, Spain





7.9. Thesis

PhD Thesis

"Micromechanics of porous and fiber-reinfored elastomers"
Student: J. Moraleda
Polytechnic University of Madrid
Advisors: Dr. J. Segurado and Prof. J. LLorca
Date: 2009

"Study of the influence of the morphology and the powder size distribution in the processing of Cu and Ni based alloys by MIM technology"
Student: J.M. Contreras Andújar
Carlos III University of Madrid
Advisors: J.M. Torralba and A. Jiménez Morales
Date: 2008

"Development of master alloys by mechanical milling for low alloy steels modification"
Student: J.A. Sicre Artalejo
Carlos III University of Madrid
Advisors: Prof. J.M. Torralba and Prof. M. Campos Gómez
Date: 2009

thesis

Master/Bachelor Thesis

"Nanoindentación for in-situ characterization of composites"
Student: Carlos Cabeza Barrantes
Polytechnic University of Madrid
Advisors: M. Rodríguez and Dr. Jon Molina-Aldareguía
Date: 2009

"Numerical simulation of deformation mechanisms of Magnesium alloy AZ31B"
Student: Ana Fernández Blanco
Polytechnic University of Madrid
Advisors: Dr. A. Jerusalem and Dr. M.T.Pérez-Prado
Date: 2009

"The effect of ARB processing on the strain rate sensitivity of the pure Zirconium"
Student: Arcadio Varona Caballero
Polytechnic University of Madrid
Advisors: Dr. M.T. Pérez-Prado and Dr. I. Sabirov
Date: 2009

"Simulation of bird impact in composite structures"
Student: Juan Antonio Sandoval Boluda
Polytechnic University of Madrid
Advisor: Dr. C. González
Date: 2009

"Tensile mechanical behavior of ultrafine grain size Zr"
Student: Zuriñe Aranguiz Merchán
Polytechnic University of Madrid
Advisor: Dr. M.T. Pérez-Prado
Date: 2009

"Mechanical and microstructural characterization of pure Zr processed via high pressure torsion"
Student: María José Vera
Polytechnic University of Madrid
Advisor: Dr. M.T. Pérez-Prado
Date: 2009

7.10. Internships

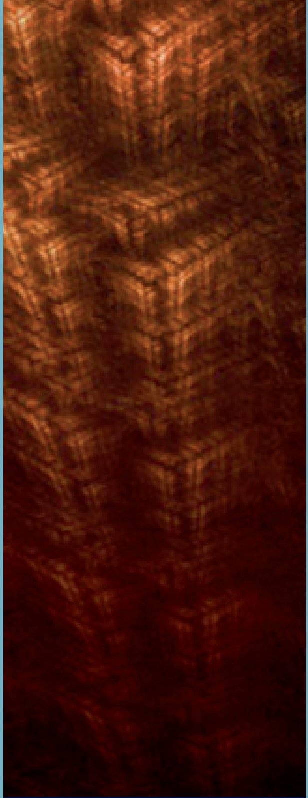
"Development of segmentation techniques of biological/medical images for biological and bioengineering continuum modeling"
Student: Mashaal Sohail
Massachusetts Institute of Technology
Supervisor: Dr. A. Jerusalem
Date: 2009

"Development of constitutive model interface between Alya and commercial softwares"
Student: Vibin Kundukulam
Internship Massachusetts Institute of Technology
Supervisor: Dr. A. Jerusalem
Date: 2009

"Manufaturing of materials by Resin Transfer Molding (RTM)"
Student: Juan José Torres
University of Navarre
Supervisor: Dr. C. González
Date: 2009-2010

"Study of the manufacturing procedure of C-fiber composites by fabric impregnation using pultrusion"
Student: Rainer Eberle
Zurich University of Applied Sciences (in collaboration with UPM)
Supervisor: Dr. C. González
Date: 2009-2010

internships



8 scientific highlights

new routes for

New routes for new materials

Throughout history, mankind has struggled to develop materials with advanced properties and this effort has contributed to continuous increases of the living standards. However, major current challenges such as sustainable growth, a fair distribution of resources (water, food), and better health care for everyone require a continuing effort in materials innovation. Many approaches have been tried in the past to manufacture new materials. In the realm of structural applications, new materials in bulk form were obtained by changing the chemical composition, modifications of the microstructure through sophisticated thermo-mechanical treatments, making composites (metal-metal, metal-ceramic, metal-polymer) or combinations of the former. These strategies have permitted wide variations of microstructural parameters such as the crystalline structure, the grain size and shape as well as their spatial distribution, size and shape of the second phase particles, etc. In turn, these changes result in tremendous variations of the properties (mechanical, magnetic, electrical). However, the methods explained above have limitations and novel materials ask for new processing routes.

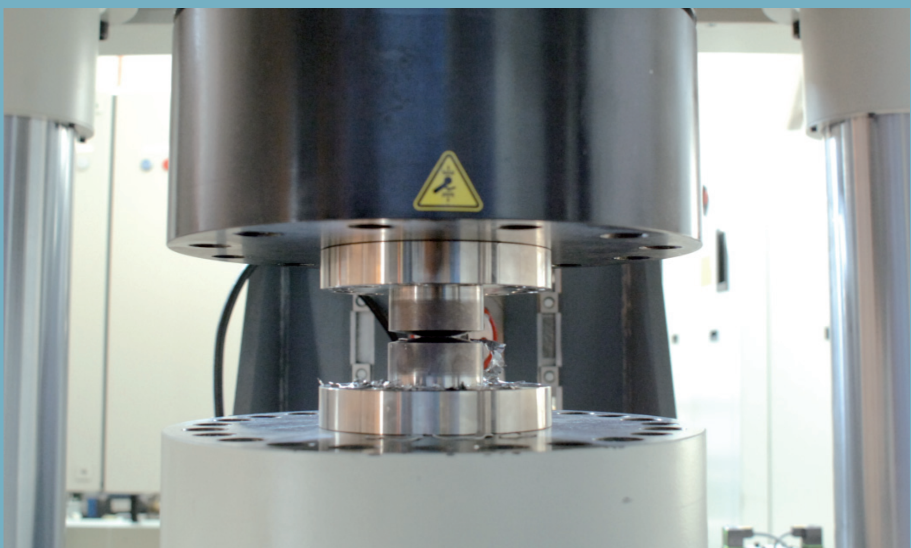


Figure 1. High-pressure torsion apparatus to manufacture novel metastable metallic phases through the simultaneous application of pressure and shear.

new materials

(a) (b)

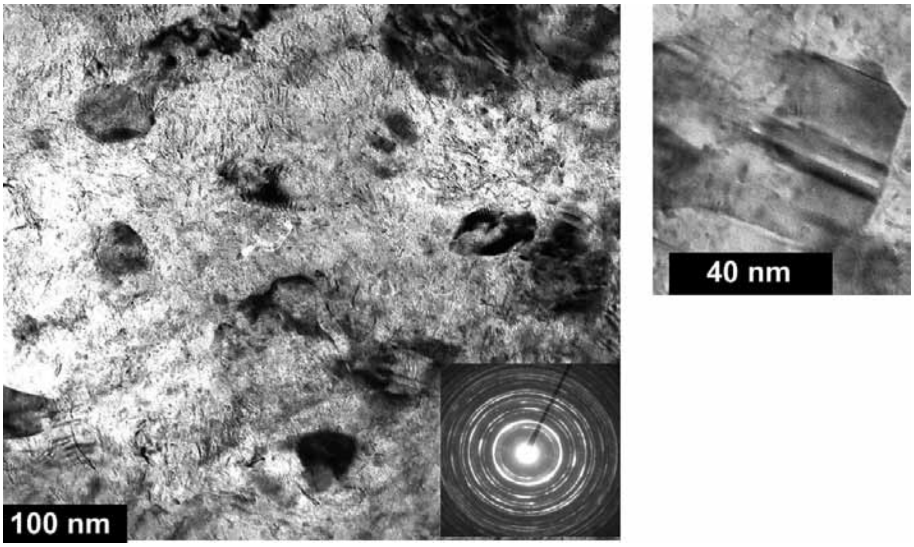


Figure 2. Omega + beta nanocrystalline pure Zr fabricated by high-pressure torsion. (a) General view, SAD pattern; (b) Nanograin showing different variants of the transformed phase.

IMDEA Materials´ scientists have recently discovered a novel processing strategy to stabilize phases of transition metals which so far could only be obtained under very high pressure at ambient conditions [1]. Through the simultaneous application of compression and shear stresses in a disk-shaped sample using a rotating plunger (Figure 1), they have been able to stabilize nanostructured omega + beta phases of pure Zr (Figure 2). Beta Zr could so far only been obtained under 30 GPa of hydrostatic pressure and it would transform back upon unloading. It has been verified that the superposition of shear deformation on top of hydrostatic pressure stimulates the phase transformation so it takes place at lower pressures and the transformed phases remain stable when the pressure is released.

Obviously, this new processing route can be applied to many metallic systems with allotropic phases that are stable only at high temperature or high pressure [3] and that are endowed with unique properties that cannot be currently exploited, opening a novel route to develop new materials with unforeseen physical properties.

[1] A.P Zhilyaev, M.T. Pérez-Prado, A. Sharafutdinov, Patent Nr. P200901060, Spain. PCT/ES2010/070017.
[2] M.T. Pérez-Prado and A.P. Zhilyaev, Physical Review Letters 102 ,175504, 2009.
[3] A.P. Zhilyaev, A. Sharafutdinov, M.T. Pérez Prado. Advanced Engineering Materials, 12, 2010. In press.

X-Ray comput

seeing is believing

Seeing is believing: X-Ray computed tomography

Polymer matrix composites are currently used in many structural applications that require a significant reduction in weight for energy and/or environmental reasons. However, despite all existing information and actual knowledge about these materials, their complex mechanical behaviour (highly non-linear, anisotropic and with different and novel failure mechanisms not found in traditional structural materials) requires greater research efforts to optimize their performance and take advantage of their full potential [1-2].

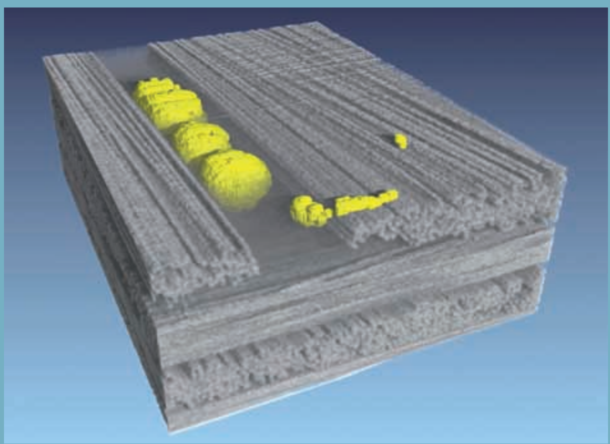


Figure 1. X-ray tomography analysis of the microstructural defects (Internal porosity in yellow) in a cross-ply glass-fibre epoxy-matrix composite (F. Sket).

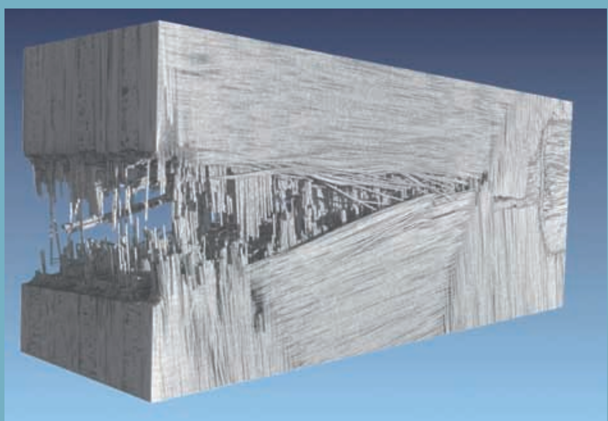


Figure 2. Deformation and fracture micromechanisms in front of a notch in a cross-ply glass-fibres epoxy-matrix composite (F. Sket, R. Seltzer, J. M. Molina-Aldareguía).

ed tomography

These efforts pass through the understanding of the effect of manufacturing defects in the final mechanical properties and through the study of their failure mechanisms. IMDEA Materials contributions in these directions are based in the application of state-of-the-art, non-destructive, three-dimensional characterization methodologies, such as X-ray computed nanotomography. This technique is based on the computer-assisted reconstruction of three-dimensional bodies based on X-ray radiographies taken from various viewing angles. The development of new X-ray generation and detection techniques allow nowadays to achieve sub-micrometer resolutions, making this technique a valuable tool for studying the complex microstructure of advanced materials as well as the dominant fracture mechanisms. Moreover, three-dimensional images can be used to perform detailed quantitative analysis of microstructural features or used as input to model which take into account the actual material microstructure to predict the macroscopic mechanical behaviour.

[1] E. Totry, C. González, J. LLorca. Composites Science and Technology 68, 3128-3136, 2008.
[2] E. Totry, C. González, J. LLorca, J. Molina-Aldareguía. International Journal of Fracture 158, 197-209, 2009.
[3] A. Enfedaque, J. M. Molina-Aldareguía, F. Gálvez, C. González, J. LLorca. Journal of Composite Materials, 44, 2010. In press.

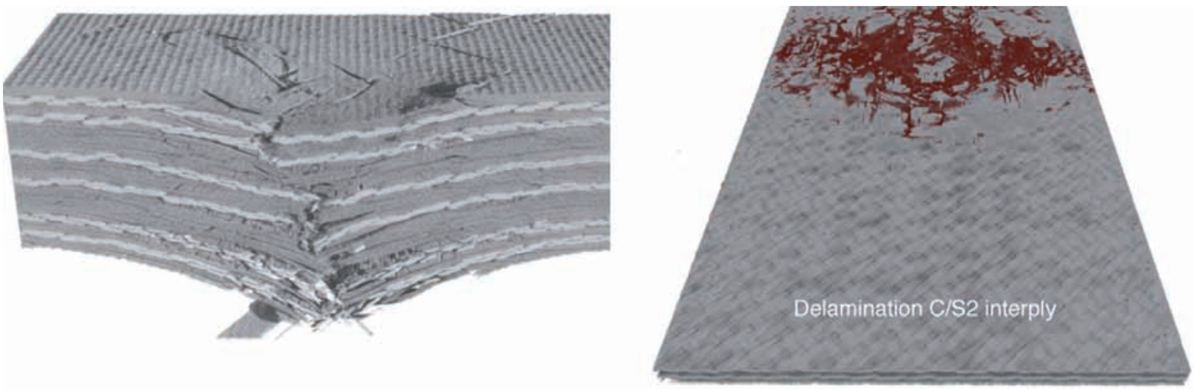


Figure 3. X-ray tomography sections of a glass-carbon fibre hybrid composite laminate subjected to out-of-plane low velocity impact with 63 J. (a) Cross-section under the impact axis, showing tensile fracture of the bottom plies and crushing of the top plies under the tup. The intraply cracks in the bottom and top plies grew upwards and downwards, respectively, leading to the development of delamination cracks, and final fracture took place by the formation of a crack through the laminate thickness. (b) Cross-section parallel to the lamina, showing the extent of delamination at the interply between carbon and glass fibre lamina [3].

breaking very

Breaking very small things ...

Constitutive equations are mathematical models that describe the mechanical behaviour of materials until rupture. They are necessary in the component design and validation processes and, in particular, they are critical to predict failure and assess the structural integrity. Accurate constitutive models of "simple" materials have been developed and validated over the years. Current trends to reduce weight and energy consumption and increase functionality, are, however, leading to the development of "complex" materials with unconventional microstructures (multifunctional composites, nanostructured metals, etc. [1-2]) or materials with evolving microstructures which deform by unconventional mechanisms (TRIP and TWIP steels [3]). Most existing constitutive models fail to reproduce their mechanical behaviour because they are not able to capture the essential features of the mechanisms of deformation and fracture in the nm-µm range. Therefore, understanding the microstructure evolution under mechanical loading at the microscopic level is essential to improve the structural integrity and reliability of components.

To explore the deformation and fracture mechanisms of materials in the nm-µm range, IMDEA Materials' research line on Advanced Characterization of Materials has developed the capability to perform in-situ mechanical tests inside scanning electron. Moreover, full-field measurements of the strains in the different phases of complex materials can

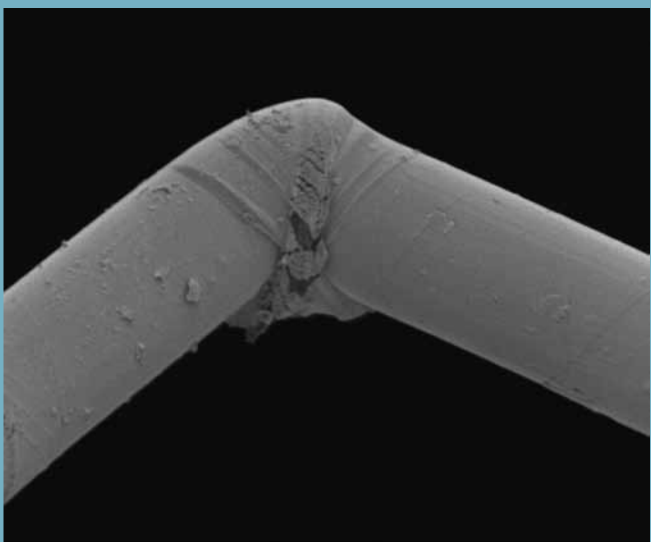


Figure 1. Failure by fibre kinking under compression of a high strength PBO fiber (K. Tamargo, J. M. Molina-Aldareguía, C. González and J. LLorca).

small things...

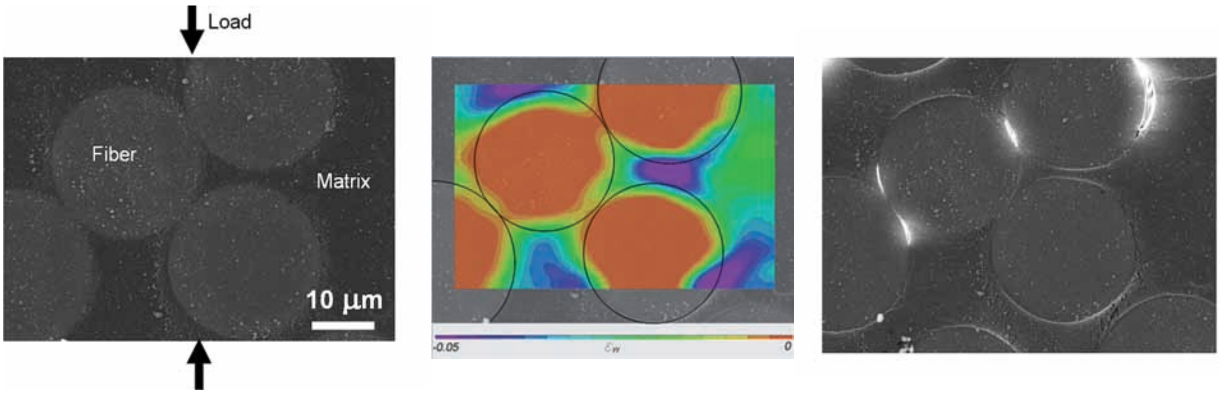
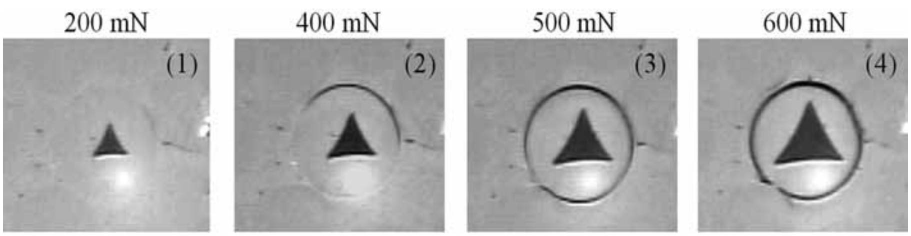


Figure 2. Deformation and fracture in uniaxial compression of a glass-fibre epoxy matrix composite inside the scanning electron microscope. (a) Secondary electron image showing fibres and matrix distribution. (b) Strain field (superimposed on the previous image), showing the strain concentration in the matrix. (c) Onset of fracture through interface decohesion (J. M. Molina-Aldareguía, L. P. Canal and C. González).

be obtained from the analysis of the micrographs using digital image correlation. This technique offers the possibility to visualize the evolution of the microstructure under mechanical load, to follow the way the stresses are shared between the different phases at the micro and nanoscale and to capture the dynamics of the deformation and fracture processes. Information obtained with these tests is complemented through instrumented nanoindentation, which provides information about the properties of the phases and interfaces in the material in the critical range from nm to µm.

[1] A. Dasari, Z.-Z. Yu, Y.-W. Mai. Polymer 50, 4112-4121, 2009.
[2] I. Sabirov, M.R. Barnett, Y. Estrin, I. Timokhina, P.D. Hodgson. International Journal of Materials Research 100, 1679-1685, 2009.
[3] M.J. Santofimia, J.G. Speer, A.J. Clarke, L. Zhao, J. Sietsma, Acta Materialia, 57, 4548-4557, 2009.
[4] J. M. Molina-Aldareguía, M. Rodríguez, C. González, J. LLorca. Philosophical Magazine, 90, 2010. In press.

Figure 3. Progressive interface fracture in a glass-fibre reinforced composite during a push-in test to assess interface strength [4]. (M. Rodriguez, J. M. Molina-Aldareguía, C. González and J. LLorca).

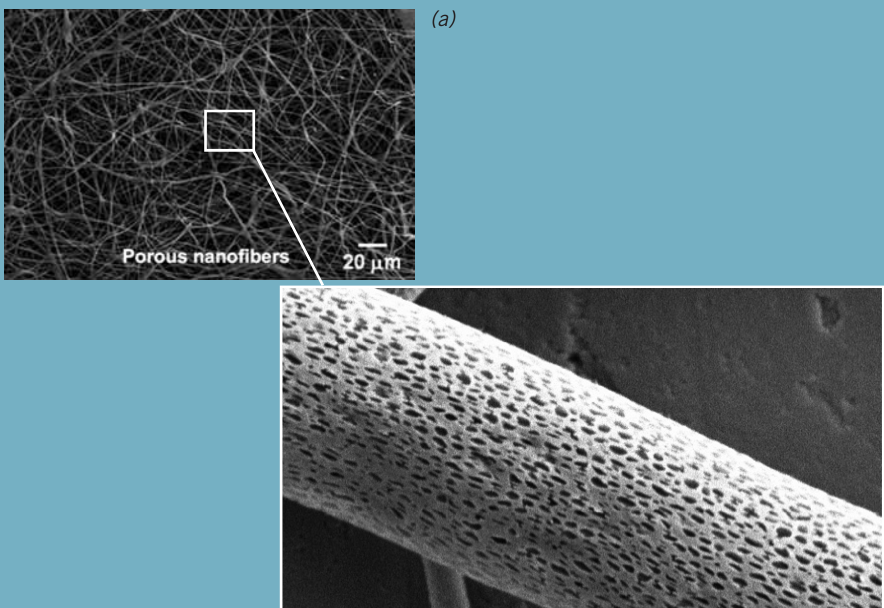


Nano-manufacturing of multifunctional ultrathin fibres

Electrospinning, a top-down nanomanufacturing process, enables production of continuous fibres ranging from nano- to sub-micron level from polymer solutions/melts in high electric fields. This process in combination with sol-gel chemistry can also produce continuous ceramic nanofibres. Added to these, the implementation of coaxial spinning allows a single-step fabrication of coated/hollow nanofibres. Depending on the type of collector, non-woven mats, aligned fibre mats and aligned fibre bundles can be fabricated. Thus, electrospinning provides a comprehensive nanomaterial and nano-manufacturing platform for a broad variety of applications like tissue engineering, filtration, protective clothing, catalysis, electronics, drug delivery and biosensors.

IMDEA Materials is currently using this technology in combination with nanoparticles in four diverse areas:

- Water treatment/purification: the objective is to achieve high flux and low fouling membranes to incorporate in a cross-flow filtration device. Functional nanoparticles (like N-doped TiO_2, TiO_2/Ag/Cu functionalized sepiolites) having photocatalytic and biocidal activities will be incorporated in hydrophilic polymer membranes. Easy access to functional nanoparticles will be granted by fabricating hollow/porous nanofibres and placing the former in the latter's core.



(a)

(b)

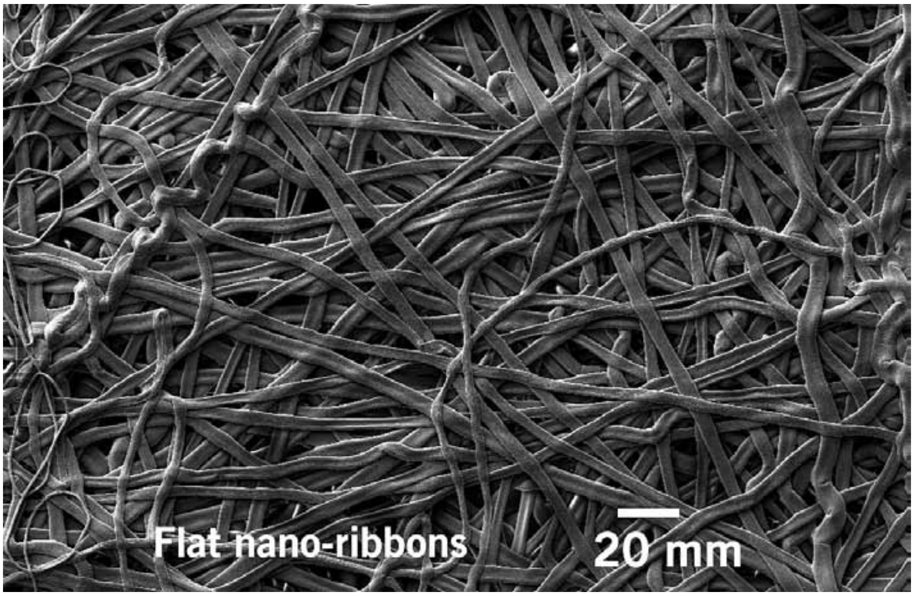


Figure 1. (a) Example of electrospun polylactid acid nanofibrous membrane with interspersed voids; the inset reveals the porous structure of individual fibres. (b) Representative example of a polymeric membrane with flat nano-ribbons. Depending on the vapour pressure/volatility of the solvents, voltage and distance between the needle and collector in spinning, different structures can be achieved to suit the application needs.

- Wound dressing: the aim of this project is to develop novel alternate biocompatible wound dressing materials, which can exhibit the required combinatorial properties like absorb exudate, maintain moist environment, adsorb odour causing molecules, permeable to oxygen impermeable to bacteria and biodegradable. For this purpose, porous polylactic acid nanofibrous mats reinforced with functionalized natural clay minerals are being evaluated.
- Advanced structural composites: the focus of the project is to prepare interleaves based on various polymeric materials/conductive nanoparticles and incorporate in fibre reinforced polymers using resin transfer moulding. The fundamental basis is to use the concept of interfaces to achieve multi-functionality (mechanical, acoustic and conductive properties).
- Bioceramics: the emphasis is to enhance the biocompatibility of pure Zr (implants) by coating with ZrO_2 nanofibres. Closely monitored activities include the interaction/adhesion of pure Zr and ZrO_2 fibres, interspersed void density and the enhanced surface area versus cell viability.

closing the gap

Closing the gap: atomistics and continuum models of plastic deformation

In a carbon-free economy, nuclear power will surely play a fundamental role as a clean and cost-competitive energy source. However, new-generation nuclear concepts involve temperature and irradiation conditions for which no experimental facility exists, making it exceedingly difficult to predict structural materials performance and lifetime. Although the gap with real materials is still large, advances in computing power over the last decade have enabled the development of accurate and efficient numerical algorithms materials simulations capable of probing the challenging conditions expected in future nuclear environments. One of the most important issues in metallic structural materials is the degradation of their mechanical properties under irradiation. Mechanical properties are intimately related to the glide resistance of dislocations, which can be increased dramatically due to irradiation-produced defects. Depending on the material crystal structure, perfect dislocations may split into partial dislocations leaving a stacking fault between them, as it is the case in FCC metals. These partials govern plasticity in these systems, being the interactions among them and with defects responsible for the material response under different external loading conditions.

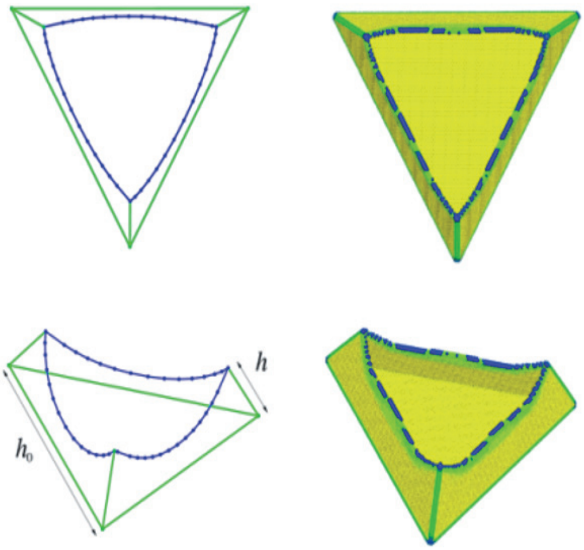
One of the main computational tools to model single crystal plasticity is called Discrete Dislocation Dynamics (DDD) which divides dislocation lines in small straight segments and solves the elastic interactions between them. Once the forces on the segment are known the position of each segment is updated according to a material dependent mobility law. We have developed a new algorithm that takes into account explicitly partial dislocations within a DDD methodology [1]. This strategy is able to follow any reaction between partials knowing at each time the right Burgers vector and the stacking fault force acting on every node. This algorithm closes the gap between atomistic calculations, where the interactions between dislocations among them and with defects are fully captured but in which the strain rate applied is too high to be realistic, and DDD with perfect dislocations in which some kind of mean field approximation has to be incorporated in order to take into account the details of those interactions.

The comparison between the results of the new algorithm and the ones obtained through the much more computationally demanding atomistic calculations are shown in Figures 1 and 2. Figure 1 presents the formation of a stacking fault tetrahedron (SFT), the most ubiquitous defect created by irradiation in FCC materials, from DDD, while Figure 2 shows the interaction between a dissociated screw dislocation and a SFT [2]. In both cases it is concluded that the algorithm is able to capture the details of the interaction while maintaining its capacity to study realistic systems. This development represents the first step to the full understanding of single crystal plasticity in materials with low stacking fault energy.

[1] E. Martínez, J. Marian, A. Arsenlis, M. Victoria and J.M. Perlado. Journal of the Mechanics and Physics of Solids, 56, 869-895, 2008,
[2] J. Marian, E. Martínez, H.J. Lee and B. Wirth. Journal of Materials Research 24, 3628- (2009) 3628.

atomistics and continuum models of plastic deformation

Figure 1. Formation of a stacking fault tetrahedron as given from an atomistic calculation and from a discrete dislocation dynamics simulation taking into account partial dislocations. On the left the results from DDD compared to the atomistic calculations on the right.



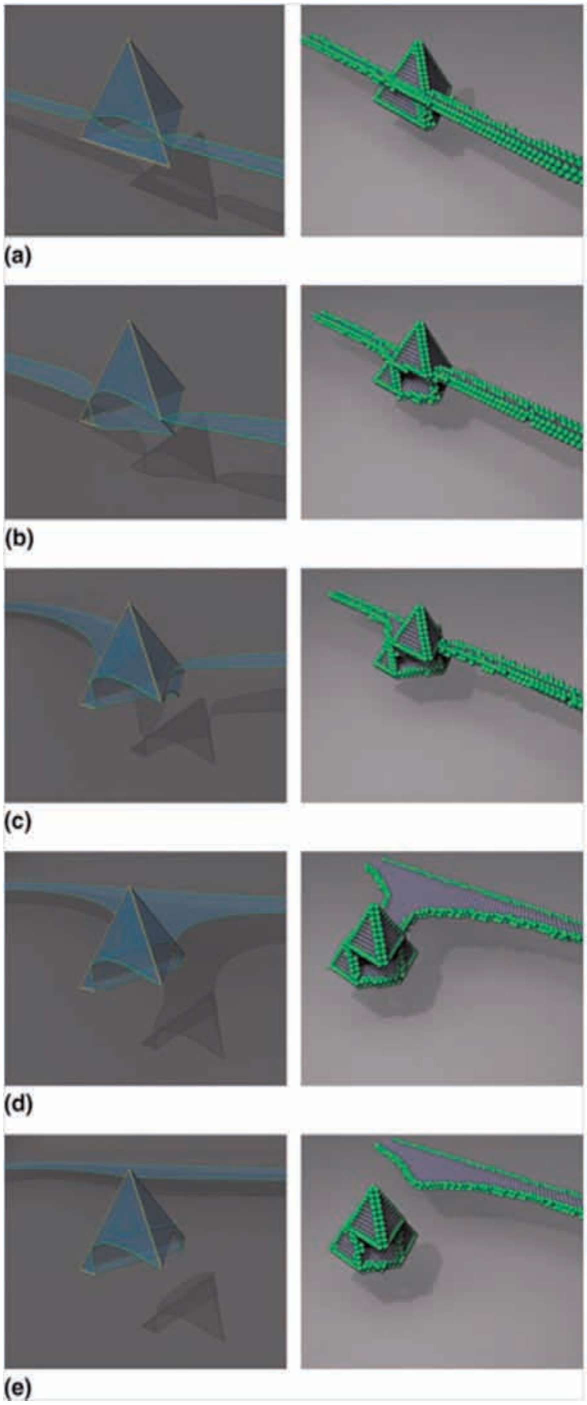


Figure 2. Comparison of the interaction of a fully dissociated dislocation and a stacking fault tetrahedron. On the left the results from dislocation dynamics are shown while the atomistic solutions are on the right.

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