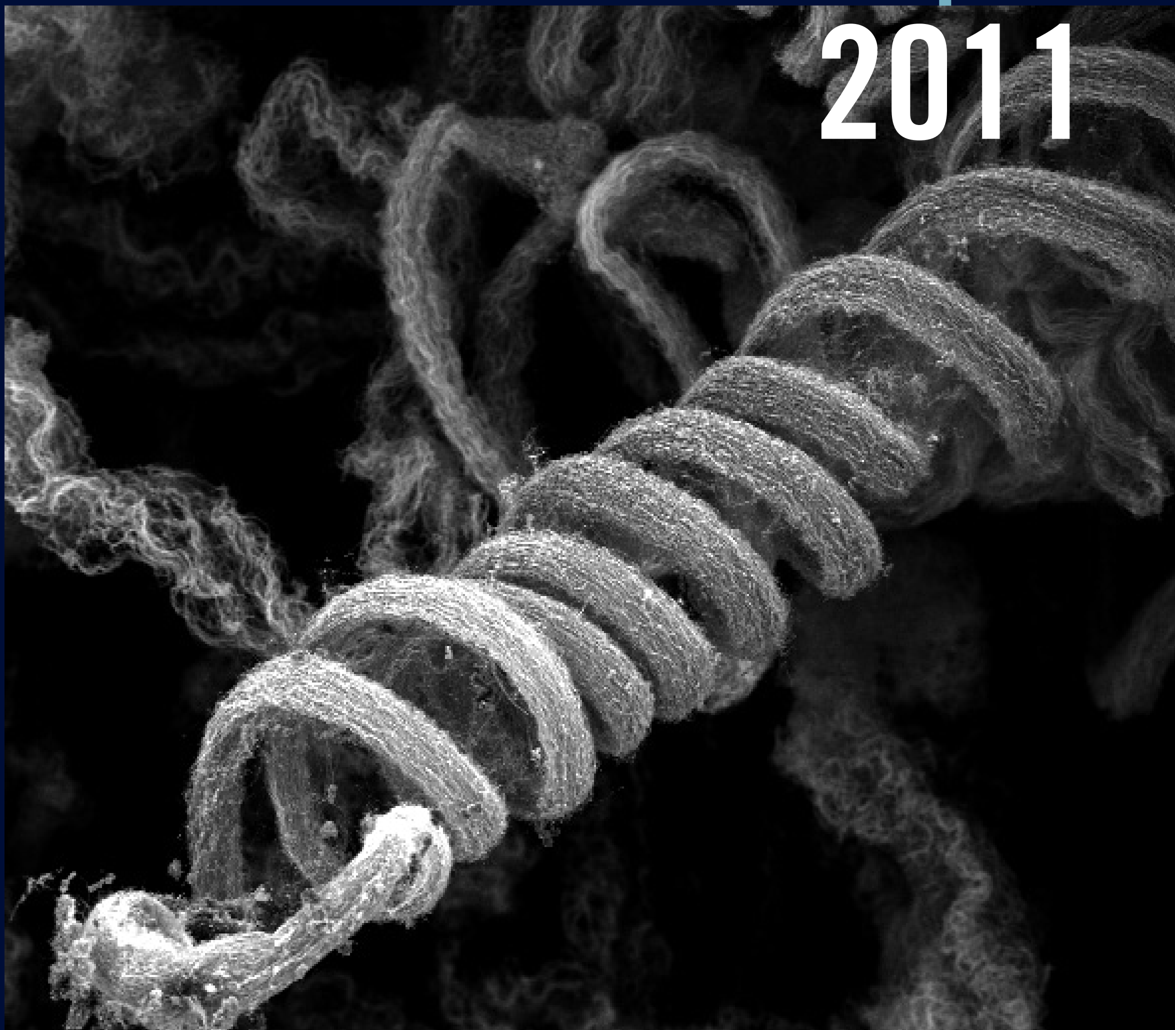
institute imdea

madrid institute
for advanced studies

institute imdea materials

annual report 2011

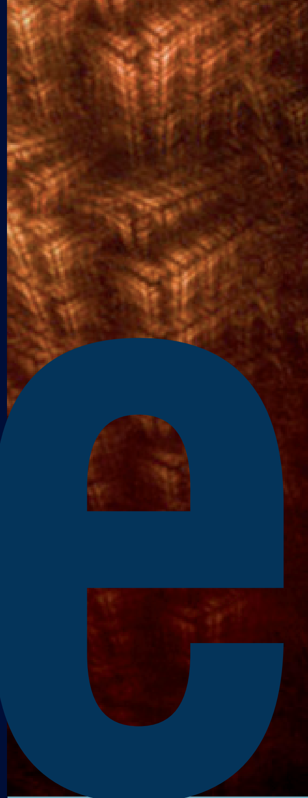


institute imdea

madrid institute
for advanced studies

institute imdea materials

annual report 2011



foreword

Javier LLorca
Director, IMDEA Materials Institute
March 2012

If the activities of IMDEA Materials Institute in 2010 were summarized in the corresponding preface to the Annual Report with the word *growth,* 2011 can be defined as the year of *consolidation.* The incorporation of three new staff researchers has completed the expertise required to compete internationally in three main areas: advanced metallic materials, structural composites with multifunctional capabilities, and modelling and characterization. With 49 researchers from 15 different countries, IMDEA Materials Institute has been faithful to its mission to attract talented people to Madrid, including Spaniards who have spent many years abroad. The Board of Trustees was also strengthened with the incorporation of two new scientific trustees, Prof. T. W. Clyne (University of Cambridge) and Prof. D. Raabe (Max-Planck-Institut für Eisenforschung), whose international reputation in our areas of expertise will help to steer the Institute in the right direction.

The construction of the building has progressed as expected and almost reached completion by the end of 2011. Construction works will be completed by March, 2012 and everybody is looking forward to relocating to the new facilities in spring. In particular, the new laboratories devoted to processing of advanced structural materials and multifunctional nanocomposites, microstructural and thermo-mechanical characterization, nanomechanics, and nanoreinforcement synthesis will boost the potential of the Institute to engage in ambitious endeavours.

As part of the science and technology system in Spain, IMDEA Materials cannot and should not ignore the current economic crisis and this has led to two main actions. On the one hand, the Institute has reinforced the links with its strategic Spanish industrial partners. Collaborations with Airbus, Gamesa and Future Fibres have been strengthened with new contracts while new partnerships were started with other Spanish companies as Acciona Infraestructuras. On the other hand, IMDEA Materials has signed the first research contracts with multinational companies established overseas (Synopsys in California and Global Foundries in Singapore), beginning the international expansion of the Institute. Moreover, four new European projects began in 2011 and, all in all, IMDEA Materials has been involved in 35 research projects, 15 of which were launched in 2011. These activities led to an increase of 47% in the competitive and industrial funds attracted by the Institute with respect to 2010.

The Institute´s research output is indicated by publications in peer-reviewed international journals (36), patents (4), plenary (11) and oral (57) presentations in international conferences, invited seminars (16) at universities and research centres and international conferences and workshops (9) organized by the Institute staff. These figures show that IMDEA Materials Institute is progressing swiftly towards the goals of excellence in research and technology transfer to industry within a truly international environment.

Last, but not least, the continuous support of the Regional Government of Madrid has to be acknowledged as the foundation of the Institute success.

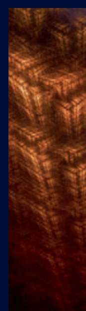
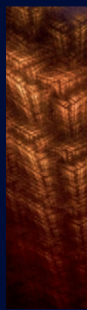
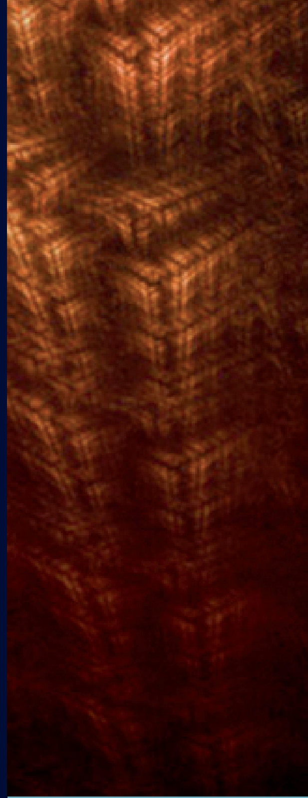


table of contents

contents



1 introduction



1.1. Profile

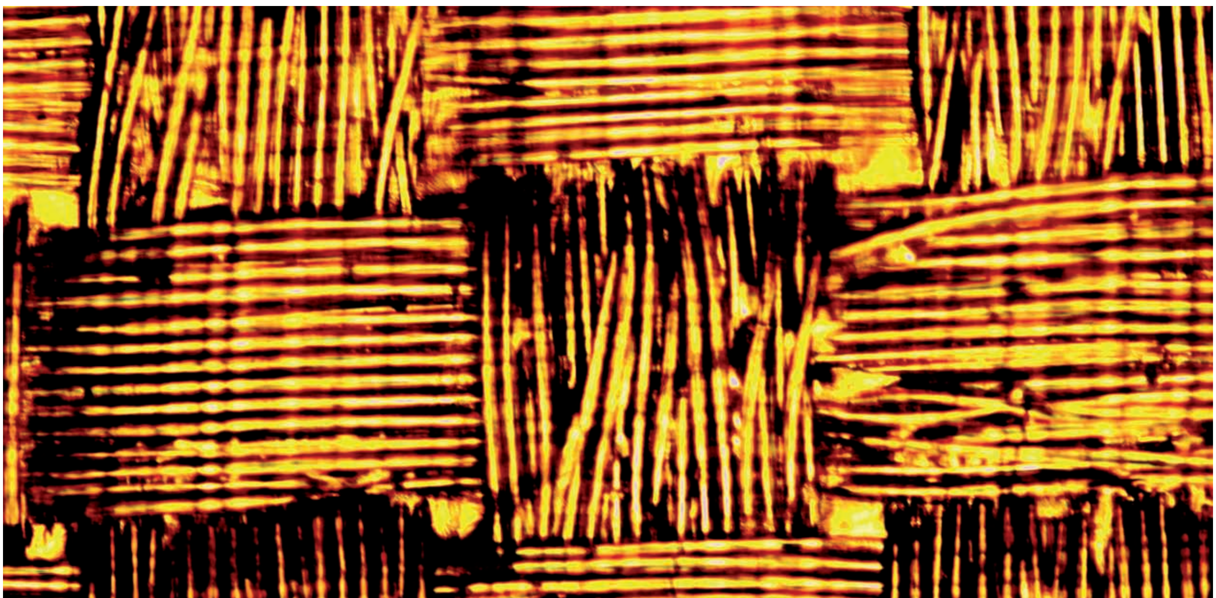
IMDEA Materials Institute is a non-profit independent research institute promoted by the Madrid regional government to perform research in Materials Science and Engineering. The Institute belongs to the Madrid Institute for Advanced Studies network, a new institutional framework created to foster social 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).

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

1.2. Appointments to the Board of Trustees and Scientific Council

Dr. Jorge Sainz, Deputy General Director for Research of the Madrid Regional Government replaced to Mr. José Manuel Pradillo Pombo as one of the permanent trustees from the Comunidad de Madrid.

Prof. T. Pinnavaia resigned as member of the Board of Trustees and of the Scientific Council in compliance with the requirements of his new position as Chief Science Officer and Executive Vice-President of InPore Technologies. He was replaced by Prof. Trevor William Clyne, Head of the Composites and Coating Group at Cambridge University. Prof. Clyne was already a member of the Scientific Council.



Prof. S. Suresh resigned as member of the Board of Trustees and of the Scientific Council in compliance with the requirements of his new position as Director of the National Science Foundation of the USA. He was replaced in both positions by Prof. Dierk Rabe, Director of Max-Planck Institut für Eisenforschung. Prof. Raabe is a scientist of international renown in the field of Physical Metallurgy and Metal Physics.

The current members of the Board of Trustees and the Scientific Council of IMDEA Materials Institute after these changes are listed in the Governing Bodies section.

1.3. Management structure

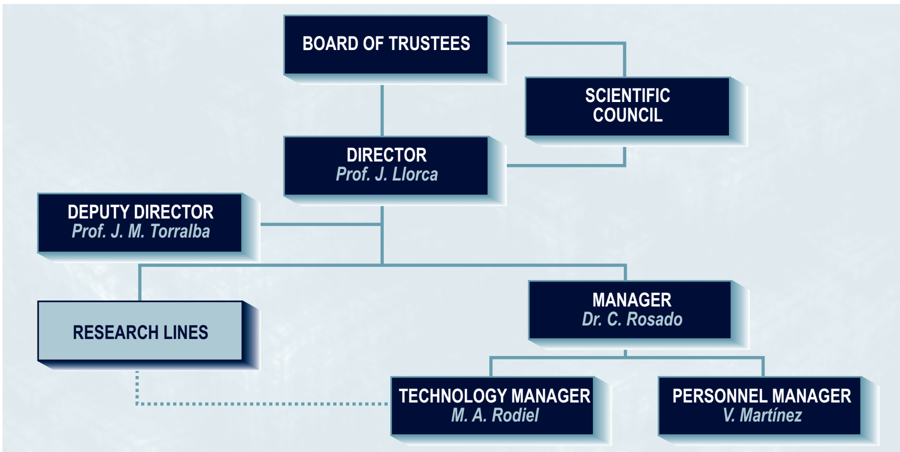


Figure 1. Current Management Structure of IMDEA Materials Institute

1.4. Headquarters building

The construction of the headquarters of IMDEA Materials Institute, located in the scientific and technological park of TecnoGetafe, is almost finished. Construction will be completed by March 2012, and personnel and equipment will move to the building in spring. The research activities in the new building are expected to start in May 2012.

TecnoGetafe, a scientific and technological park created by a joint venture of the Madrid regional government and the municipality of Getafe, is located sixteen kilometres south of Madrid. With an area of close to 1 million square meters, it is one of the largest in Europe and its activities are focussed in the areas of aerospace/aeronautics, engineering, energy and new technologies. Together with industrial enterprises, such as Sertec and Centum Solutions, TecnoGetafe also hosts FIDAMC (composite materials research centre from EADS) and the Scientific and Technological Park of the Polytechnic University of Madrid. This Scientific and Technological Park includes the university researcher centres on aerospace engineering, industrial engineering, as well as earth, energy and materials engineering and Centesil, a pilot plant devoted to the purification of silicon for photovoltaic solar cells.

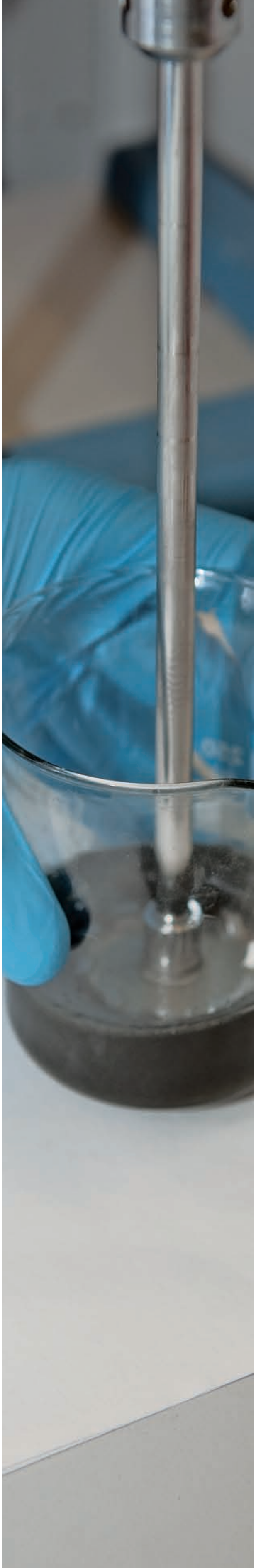
Until the new building becomes available, IMDEA Materials Institute is developing its activities in two provisional sites. The first one is located at the School of Civil Engineering of the Polytechnic University of Madrid and hosts the offices for the director and the research activities on composite materials as well as modelling & simulation. The second one, located at the Carlos III University of Madrid, hosts the research groups focused in metallic materials, multifunctional nanocomposites and advanced characterization techniques.

Figure 2. Current state of the construction of the final site of IMDEA Materials Institute in the Scientific and Technological Park of the UPM in Tecnogetafe.*

** This project has been funded by: (i) the Ministry of Science and Innovation (MICINN) within the National Plan for Scientific Research, Technological Development and Innovation 2008-2011 with record number of PCT-420000-2009-9, and (ii) through an agreement signed between MICINN, Madrid Regional Government and IMDEA Materials Institute, within the Regional Competitiveness and Employment Objective for the period 2007-2013, by the European Regional Development Fund.*

1.5. Governing Bodies

1.5.1. Members of the Board of Trustees



1.5.2. Members of the Scientific Council

Prof. John E. Allison
Professor
University of Michigan, USA

Prof. Brian Cantor
Vice-chancellor
York University, UK

Prof. Trevor W. Clyne
Professor
Cambridge University, UK

Prof. William A. Curtin
Director. Institute of Mechanics
Professor
Ecole Federale Polytechnique of Lausanne, Switzerland

Prof. Manuel Elices
Professor
Polytechnic University of Madrid, Spain

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

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

Prof. Yiu-Wing Mai
Director, Centre for Advanced Materials Technology
Professor
University of Sydney, Australia

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

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

Prof. Pedro Muñoz-Esquer
Independent consultant

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

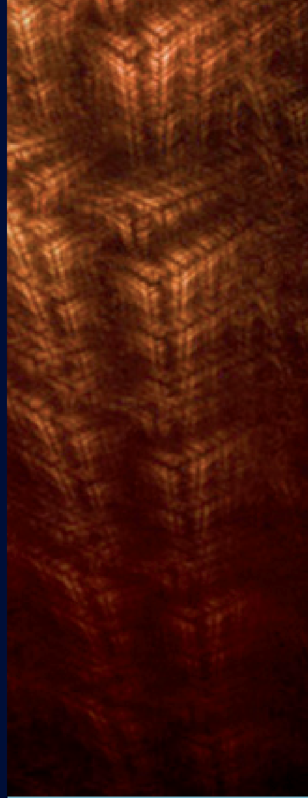
Prof. Gary Savage
Independent consultant

Prof. John R. Willis
Professor
Cambridge University, UK

Prof. Dr. Dierk Raabe
Director, Max-Planck Institute for Iron Research
Professor
RWTH Aachen University, Germany

2

industrial partnership

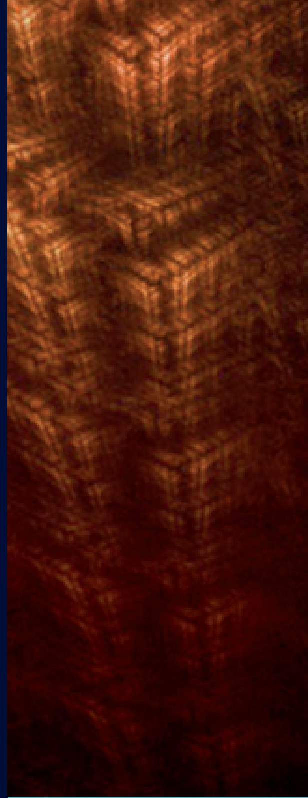


Scientific knowledge generated in research centres, such as IMDEA Materials, is critical for the increase in competitiveness of industrial enterprises in the current global and dynamic market. The transfer of knowledge and technology from IMDEA Materials to industrial partners is mainly performed through R&D collaborations in the framework of direct industrial contracts and competitive collaborative projects funded by national and international public bodies. The main industrial partners are shown in Figure 3.

Concerning industrial contracts, the 2011 budget has increased by 44% with respect to 2010. Existing strategic collaborations with Airbus, Gamesa and Future Fibres have been strengthened with new contracts, while the network of industrial partners has been extended. New research collaborations were started with Spanish companies (Acciona Infraestructuras) and IMDEA Materials has expanded its industrial links beyond Europe. Contracts were signed in 2011 with Synopsys (Mountain View, California, USA), one of the largest companies in the design of an application-specific integrated circuits, and Global Foundries (Singapore), the world's third largest independent semiconductor foundry. Internationalization of our portfolio of partners, together with the development of stronger links with Spanish strategic partners, stands as key features of IMDEA Materials' roadmap for industrial collaboration.

Figure 3. Current industrial partners of IMDEA Materials Institute

3 research



3.1. Research Groups

The Institute´s research activities are carried out within sixteen research groups led by staff Researchers. Most of the research projects are multidisciplinary and involve collaboration with different groups. The research activities are divided in three main areas. Five groups are devoted to Metallic Materials, while another five are focused on Composite Materials and six groups provide transversal support on Modelling and Characterization to all the groups. The staff researchers and the corresponding research lines are shown in Figure 4.

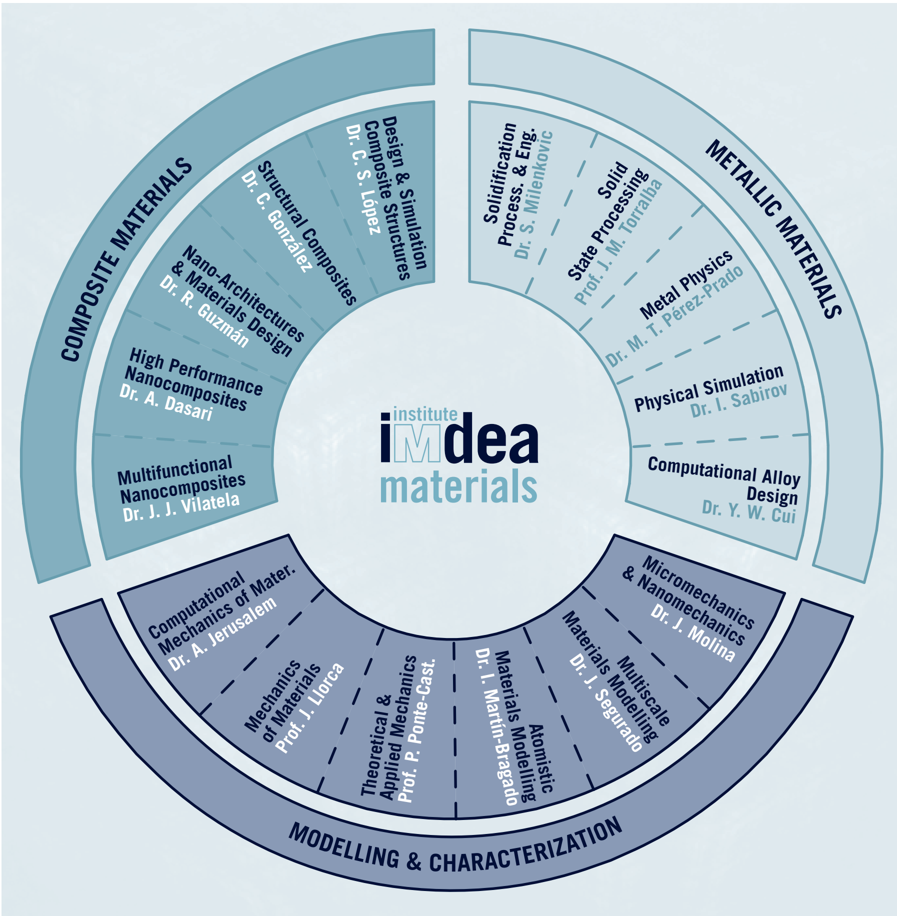


Figure 4. Research groups of IMDEA Materials Institute

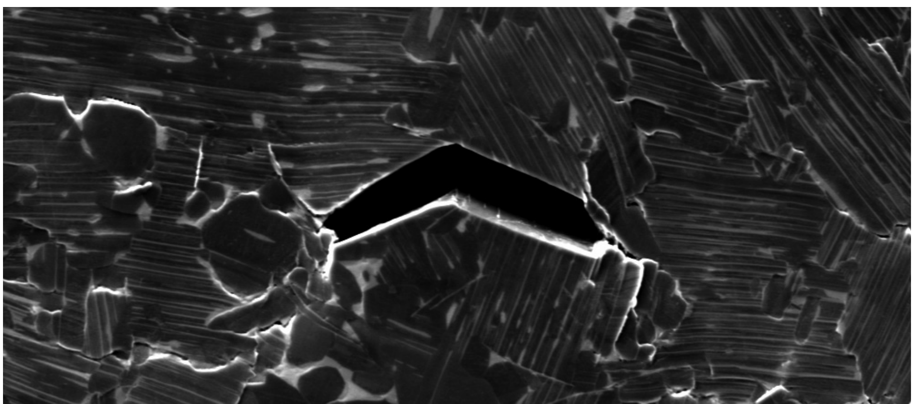
3.1.1. Modelling & Characterization

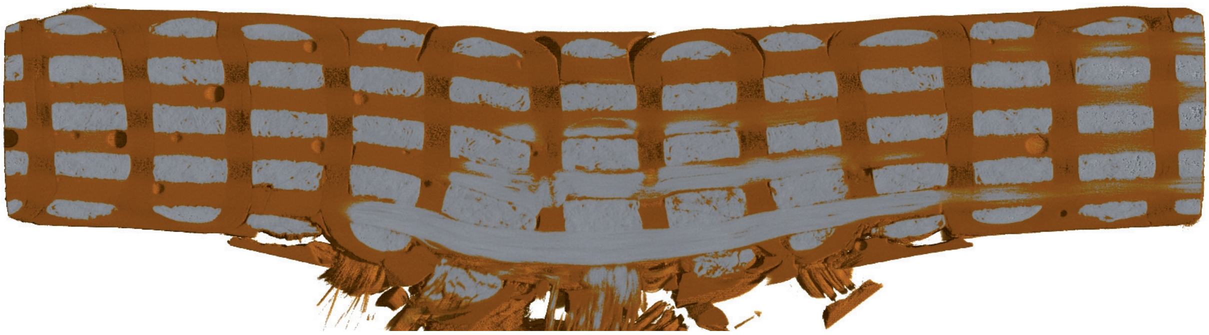
The modelling activities of the Institute are carried out by five research groups: **Mechanics of Materials** (Prof. J. LLorca), **Theoretical and Applied Mechanics** (Prof. P. Ponte-Castañeda),

Computational Mechanics of Materials (Dr. A. Jérusalem), **Multiscale Materials Modelling** (Dr. J. Segurado), **Atomistic Materials Modelling** (Dr. I. Martin-Bragado). The groups focused on the modelling activities bring together expertise that 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. The main research activities are related to the development of advanced tools and simulation strategies to carry out virtual tests of composites and metallic materials, the prediction of size effects in the mechanical behaviour at the nm-μm scale, the development of homogenization estimates for non-linear composites, and the understanding the behaviour and structural evolution of neurons upon mechanical loading. These modelling efforts are complemented with the activities of the **Nanomechanics and Micromechanics** (Dr. J. M. Molina-Aldareguía), whose leading objective is to develop novel experimental methods to quantify mechanical properties at the nm-μm scale, in addition to the application of state-of-the-art techniques for microstructural characterization (TEM, SEM, X-ray diffraction, TGA, DSC, spectroscopy, etc.). Current activities in this group include the analysis of the deformation and fracture mechanisms in structural composites and metallic alloys at ambient and elevated temperatures by means of *in situ* mechanical tests in scanning electron and/or atomic force microscopes, the development of testing methodologies to measure *in situ* matrix and interface mechanical properties in composites, the experimental determination of size effects on the flow strength of ceramic nanopillars, and the characterization of defects and voids at the microscale by means of X-ray computer-assisted microtomography.

3.1.2. Metallic Materials

The activities of IMDEA Materials in the area of Metallic Materials are distributed between five research groups devoted to **Solid State Processing** (Prof. J. M. Torralba), **Metal Physics** (Dr. M. T. Pérez-Prado), **Physical Simulation** (Dr. I. Sabirov), **Solidification Processing and Engineering Design** (Dr. S. Milenkovic) and **Computational Alloy Design** (Dr. Y. Cui). Research activities in this line aim to establish relationships between the processing methods, the microstructure and the mechanical behaviour of a wide range of metallic materials in close interaction with the “Modelling and Characterization” groups. A large array of processing techniques for engineering alloys (including powder metallurgy, directional solidification

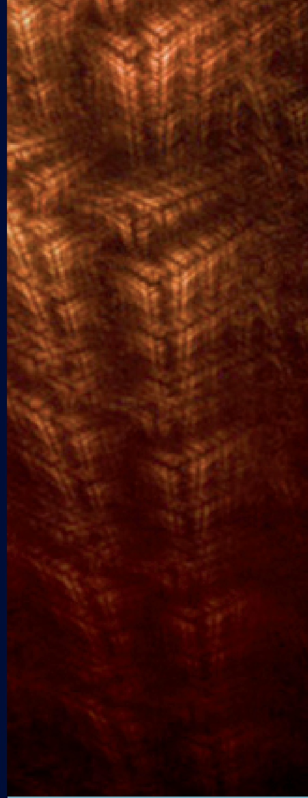




and casting, high-pressure die casting, hydrostatic extrusion, welding, severe plastic deformation, etc.) is utilized to fabricate metals with tailored mechanical properties. Microstructures are characterized by X-ray diffraction (including 3D XRD performed using synchrotron radiation), microtomography, electron backscatter diffraction (EBSD) and electron microscopy (TEM, SEM). The mechanical behaviour of materials is investigated by a combination of ex-situ as well as in-situ testing in an electron microscope. Physical simulation of the influence of processing parameters on the microstructure is carried out using a Gleeble system and new alloys with optimized properties are designed by means of computational thermodynamics. In addition, crystal plasticity finite element models are used to simulate the mechanical behaviour as well as the evolution of the texture and the interaction among the different deformation mechanisms. Materials currently under investigation include Mg alloys, ultrafine grained metals and directionally-solidified nanowires with high strength and multifunctional properties, as well as Ni-based superalloys and intermetallics for high temperature structural applications.

3.1.3. Composites

The activities of IMDEA Materials Institute in the area of composite materials are performed by five research groups: **Structural Composites** (Dr. González), **Design & Simulation of Composite Structures** (Dr. C. Lopes), **Multifunctional Nanocomposites** (Dr. J. J. Vilatela), **High Performance Nanocomposites** (Dr. A. Dasari) and **Nano-Architectures and Materials Design** (Dr. R. Guzman de Villoria). Current efforts include the optimization of out-of-autoclave processing techniques (pultrusion, resin-transfer moulding, infiltration) with special emphasis in the effect of defects, novel hybrid and 3D structural composites with enhanced mechanical properties (impact resistance), and the development of novel polymer-based nanocomposites with multifunctional capabilities (fire resistance, electrical and thermal conductivity, photocatalytic activity, etc.). Electrospun mats made up from nano- to sub-micron polymer and ceramic fibres are manufactured for a broad variety of applications like tissue engineering, filtration, protective clothing, and biosensors. In addition, in order to tailor the macroscopic mechanical and functional properties of the composites, nano-scale structures will be placed strategically inside the material. Tougher aerospace composites, enhanced non-destructive evaluation, de-icing/anti-icing capabilities, mechano-mutability are some of the envisioned properties of these new generation of materials. Finally, the design of advanced composites with non-conventional architectures and by non-conventional methods is also studied.



4

people

As stated in the mission, one of the main goals of IMDEA Materials Institute is attracting talented researchers from all over the world to the region of Madrid. 3 Staff Researchers, 5 Postdoctoral Research Associates and 8 Research Assistants joined the Institute in 2011, leading to a total of 49 Researchers, including 6 Senior Researchers, 1 Visiting Scientist, 10 Researchers, 11 Postdoctoral Research Associates, and 21 Research Assistants from 15 different nationalities. It should be noted that 55% of the researchers are foreign nationals while 71% of the Ph.D.s were granted by foreign universities. This multisdisciplinary talented group is contributing to establish IMDEA Materials Institute as an international reference in Materials Science and Engineering.

senior researchers

Prof. Javier LLorca

Director,
Mechanics of Materials

Ph.D. in Materials Science from Polytechnic University of Madrid. Spain

Professor and Head of the Advanced Structural Materials and Nanomaterials Research Group, Polytechnic University of Madrid

Research Interests

Analysis of the relationship between microstructure and mechanical properties in advanced structural materials; development of novel multiscale simulation strategies to predict the macroscopic mechanical behaviour of materials from microstructural information; and experimental characterization techniques to measure the mechanical properties of materials under extreme conditions at microscopic and macroscopic levels.

Prof. Jose Manuel Torralba

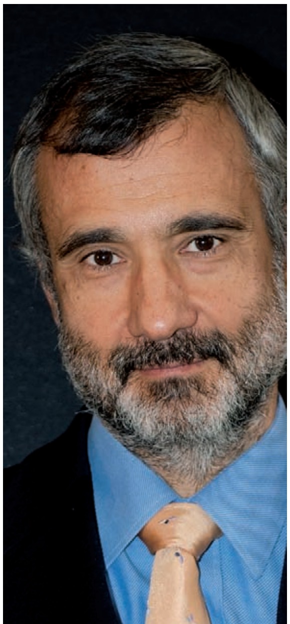
Deputy Director,
Solid State Processing

Ph. D. in Metallurgical Engineering from Polytechnic University of Madrid. Spain

Professor of Materials Science and Engineering, Carlos III University of Madrid

Research Interests

Manufacturing of advanced structural materials by powder metallurgy; 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 aluminium, iron or high speed steel; and processing technologies as mechanical alloying, metal injection moulding or spray pyrolysis to manufacture nanoparticles.



Dr. Carlos González
Senior Researcher,
Structural Composites

Ph.D. in Materials Science from Polytechnic University of Madrid. Spain

Associate Professor of Materials Science, Polytechnic University of Madrid

Research Interests
Processing, characterization and modelling (theoretical and numerical) of the mechanical performance of advanced structural materials, with special emphasis in metal- and polymeric-matrix composites; and development of physically-based, micromechanical models of the deformation and fracture (multiscale models to design novel virtual testing strategies).

Dr. Jon M. Molina-Aldareguía
Senior Researcher,
Micromechanics and Nanomechanics

Ph.D. in Materials Engineering from Cambridge University. UK

Research Interests
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. Teresa Pérez-Prado
Senior Researcher,
Metal Physics

Ph.D. in Materials Science from Complutense University of Madrid. Spain

Research Interests
Applied and fundamental work on the processing, characterization and mechanical behaviour of advanced metallic materials for automotive, energy and biomedical applications; study of the mechanical response of bulk and porous magnesium alloys, as well as the *in situ* investigation of the deformation and recrystallization mechanisms of TiAl alloys; and fabrication of novel metallic phases with improved mechanical and functional properties by severe plastic deformation involving compression and shear.

Prof. Pedro Ponte Castañeda
Associated Senior Researcher, Theoretical and Applied Mechanics

Ph.D. in Applied Mathematics from Harvard University. USA

Professor and Graduate Group Chair in the Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania

Research Interests
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.

visiting scientist

Dr. Carl Boehlert
Visiting Scientist,
Physical Metallurgy

Ph.D. in Materials Science and Engineering from University of Dayton. USA

Research Interests
Materials processing, microstructural evolution, mechanical testing and behaviour, microscopy and microstructure-property relationships of high-temperature alloys, lightweight magnesium structural alloys, and metal matrix composites.

researchers

Dr. Yuwen Cui
Researcher,
Computational Alloy Design

Ph.D. in Materials Science from Central South University. China

Research Interests
Computational thermodynamics (i.e. CALPHAD) and kinetics; high throughput diffusion research and diffusion modelling; microstructural simulation by using the Landau theory and phase field model; development of commercial thermodynamics databases and computational alloy design of Pb-free micro-solders, Ni-base superalloys and the new generation of Co-based high temperature alloys; development of lightweight interstitial alloys for hydrogen storage.

Dr. Aravind Dasari
Researcher, Multifunctional Nanocomposites

Ph.D. in Materials Engineering form University of Sydney. Australia

Research Interests
Electrospinning of multifunctional nanofibers; processing-structure-property relationships of polymeric materials and more specifically, thermal stability/flame retardancy, tribology, and deformation/fracture mechanisms of polymer nanocomposites; Development of novel multifunctional and environmentally-friendly materials.

Dr. Antoine Jérusalem
Researcher, Computational Mechanics of Materials

Ph.D. in Computational Mechanics of Materials from MIT. USA

Research Interests
Computational modelling of many types of materials and structures; 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. Ignacio Martín-Bragado
Researcher, Atomistic Materials Modelling

Ph.D. in Physics from University of Valladolid. Spain

Research Interests

Kinetic Monte Carlo simulation of diffusion and activation/deactivation of dopants in silicon and other alloys used in microelectronics; molecular dynamics and kinetic Monte Carlo simulation of damage by irradiation in structural materials for nuclear applications; development of other atomistic (*ab initio*) and multiscale simulation techniques.

Dr. Srdjan Milenkovic
Researcher, Solidification Processing & Engineering

Ph.D. in Materials Engineering from State University of Campinas. Brazil

Research Interests

Processing, solidification behaviour, mechanical and microstructural characterization, as well as processing-structure-property relationships of Ni-based superalloys, intermetallic compounds and eutectic alloys for high-temperature applications; nanotechnology in general, and more specifically, synthesis and characterization of metallic nano-wires through directional solidification and electrochemical treatment of eutectic alloys.

Dr. Ilchat Sabirov
Researcher, Physical Simulation

Ph.D. in Metallurgy from Montanuniversitaet Leoben. Austria

Research Interests

Deformation processing of metallic materials, microstructure evolution during deformation processing, and physical simulation of these processes using state-of-the-art GLEEBLE 3800 system.

Dr. Javier Segurado
Researcher, Multiscale Materials Modelling

Ph.D. in Materials Engineering from Polytechnic University of Madrid. Spain

Research Interests

Multiscale modelling of structural materials (different materials and length scales); discrete dislocation dynamics and single-crystal plasticity models to study plastic deformation of metallic materials; development of computational micro-mechanics strategies to simulate the mechanical behaviour until failure of both particle and fibre reinforced composites.

new researchers

Dr. Roberto Guzmán de Villoria

Researcher,
Nano-Architectures and Materials Design

Ph.D. in Mechanical Engineering from the University of Zaragoza. Spain

Dr. Guzman de Villoria received his M.Sc. in Physics in 2000 and his M.Eng. in Materials in 2002 from the University of Salamanca, Spain. He obtained his Ph.D. (2007) from the University of Zaragoza and, as a Ph.D. student, he pioneered the application of carbon nanotubes and nanofibers in composite materials. After his graduation, Dr. Guzman de Villoria joined the Department of Aeronautics and Astronautics at MIT as a Post-doctoral Associate, where he carried out research on novel methods of manufacturing carbon nanotubes (especially continuously) and on the mechanical and multifunctional properties of nano-engineered composites. He has been the leading post-doctoral researcher of MIT's Nano-Engineered Composite aerospace STructures (NECST) Consortium. He was awarded a Ramon y Cajal fellowship in 2012 to join IMDEA Materials Institute. Dr. Guzman de Villoria has co-authored 20 papers in international peer-reviewed journals (Advanced Materials, ACS Nano, Composite Science and Technology, Acta Materialia, etc.), holds an h-factor of 9 and has participated in various industrial research projects in the field of nano-composites, hierarchical structures and nano-engineered composites for aerospace applications. He is co-inventor of 4 international patents.

Research Interests

Nano-architectures; design and development of new materials and structures with tailored mechanical and functional properties; manufacturing new nano-engineered materials, bio-inspired materials and mechanomutable structures for transportation, energy and biomedical applications.

Dr. Claudio Saul Lopes

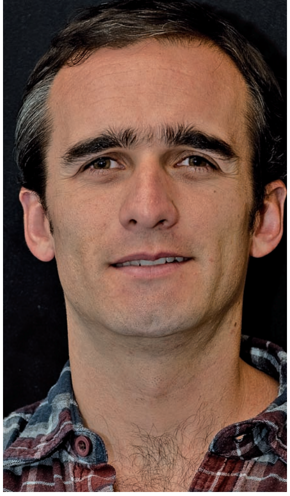
Researcher, Design & Simulation of Composite Structures

Ph.D. in Aerospace Engineering from Delft University of Technology. The Netherlands

Dr. Lopes graduated in Aerospace Engineering at the Lisbon University of Technology (2000), and holds M.Sc. (2002) and Ph.D. (2009) degrees in Aerospace Engineering from the Delft University of Technology (The Netherlands). His Ph.D. research on 'damage and failure of non-conventional composite laminates', was carried out in collaboration with the University of Porto (Portugal). After graduation, he joined INEGI, an interface institute on mechanical engineering from the University of Porto, as a Post-doctoral Researcher where he managed several projects with emphasis on composite applications for aerospace applications (design, analysis and production). He has participated in 14 researcher projects funded by EU, international agencies (ESA, NASA) and industrial enterprises companies, 8 as principal investigator. Dr. Lopes has co-authored 10 papers in international peer-reviewed journals devoted to composite materials (Composites Science and Technology, Composites A, Journal of Composite Materials, etc.). He joined IMDEA Materials Institute in June 2011 and he has been awarded the Juan de la Cierva fellowship from the Spanish Ministry of Science and Innovation.

Research Interests

Design and simulation of composite structures; design of advanced composites with non-conventional architectures and by non-conventional methods, such as fibre-steered composite panels manufactured by means of Advanced Fibre Placement; numerical analysis and computational simulation of damage and failure of composite structures; impact and damage tolerance analysis of composite structures.



Dr. Juan José Vilatela

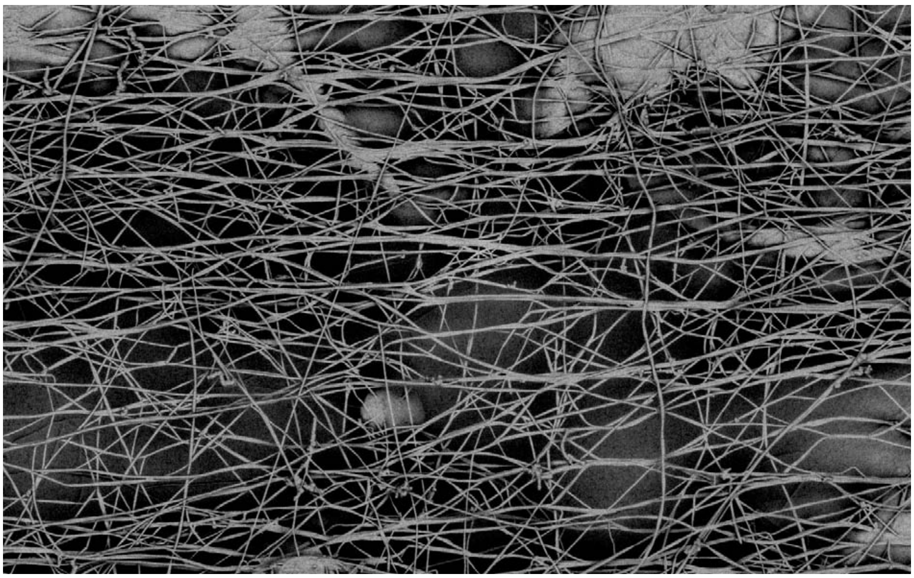
Researcher, Multifunctional Nanocomposites

Ph.D. in Materials Science from University of Cambridge. UK

Dr. Vilatela has a B.Sc (2005) in Engineering Physics (honours) from Universidad Iberoamericana, Mexico, and a Ph.D (2009) from Cambridge University. Before joining IMDEA Materials Institute, he worked as a Postdoctoral Research Associate in the Department of Materials Science and Metallurgy at Cambridge University. His research focused mainly on the development of a new high-performance fibre made of carbon nanotubes. The novel fibre spinning process is currently under industrial scale-up and Dr. Vilatela is an active consultant in this development. Dr. Vilatela has co-authored 13 papers in international peer-reviewed journals (Science, Advanced Materials, Advanced Functional Materials, ACS Nano, Composite Science and Technology, etc.) and is co-inventor of 3 patents. He joined IMDEA Materials Institute in June 2011 and he has been awarded the Juan de la Cierva fellowship from the Spanish Ministry of Science and Innovation.

Research Interests

Nanocomposite materials, produced by controlled assembly from the nano to the macroscale, where the possibility of hierarchical tailoring provides materials with multifunctional properties (e.g. mechanical, thermal), often superior to those of conventional materials, and makes them suitable for a wide variety of applications; carbon nanotubes, CNx, inorganic nanotubes (e.g. TiO_2), cellulose, grapheme and silica nanoparticles as well as thermoset, elastomeric and thermoplastic matrices; applications of Raman spectroscopy and synchrotron X-ray diffraction to study the structural evolution of materials under mechanical deformation.



postdoctoral research associates

Dr. Michalis Agoras
Postdoctoral Research Associate

Ph.D. in Mechanical Engineering and Applied Mechanics from University of Pennsylvania. USA

Research Interests
Development of homogenization methods for the determination of the finite-strain effective response of multi-scale heterogeneous systems, such as thermoplastic elastomers, in terms of the corresponding local material response of the constituent (nonlinear) phases and the underlying microstructure.

Dr. Somjeet Biswas
Postdoctoral Research Associate

Ph.D. in Materials Engineering from the Indian Institute of Science Bangalore. India

Research Interests
Processing, microstructure and mechanical properties high-pressure die cast Mg alloys; X-ray computed microtomography.

Dr. Juan Pedro Fernández
Postdoctoral Research Associate

Ph.D. in Chemistry from the Complutense University of Madrid. Spain

Research Interests
Processing and characterization of polymer-based nanocomposites; study of the effect of the nanocompounds on the structure and properties of polymer matrices.

Dr. Berta Herrero
Postdoctoral Research Associate

Ph.D. in Chemistry from Complutense University of Madrid. Spain

Research Interests
Processing and characterization of polymer nanocomposites for advanced applications; fillers for rubber formulations, organically-modified nanoclays and flame retardant additives.

Dr. Miguel Monclús
Postdoctoral Research Associate

Ph.D. in Thin Film Technology from Dublin City University. Ireland

Research Interests
Characterization and performance of coatings, multilayers and nanostructured materials by means of nanoindentation, atomic force microscopy and other advanced techniques and instruments.

Dr. Jerome Rajakesari
Postdoctoral Research Associate

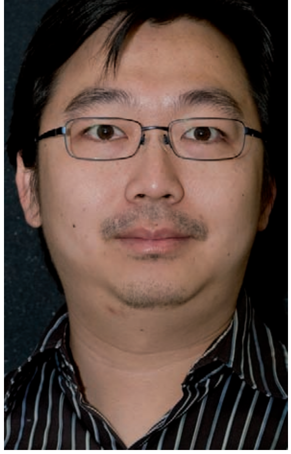
Ph.D. in Mechanical Engineering from Indian Institute of Technology Madras. India

Research Interests
Multiscale modelling of electrical conductivity of carbon-nanotube reinforced polymer-matrix composites from nm to continuum level; simulation and design of carbon-nanotube reinforced polymer-matrix composites for lightning impact applications.

Dr. Rocio Seltzer
Postdoctoral Research Associate

Ph.D. degree in Materials Engineering from University of Sydney. Australia

Research Interests
Optimization of out-of-autoclave processing techniques for advanced polymer composites; analysis of the structure/property relationships in polymer composites by means of finite element simulations and advanced three-dimensional characterization techniques; manufacturing of advanced materials by rapid prototyping.



Dr. Denny Tjahjanto
Postdoctoral Research Associate

Ph.D. in Engineering Mechanics from Delft University of Technology. The Netherlands.

Research Interests
Development of multiscale numerical models for simulating damage and failure in fiber-reinforced composite materials using state-of-the-art finite element techniques.

Dr. Raghu Raja
Postdoctoral Research Associate

Ph.D. in Chemical Engineering from Indian Institute of Technology Kharagpur. India

Research Interests
Manufacturing and product development of polymer matrix composites; process modelling and simulation and performance analysis.

Dr. Srinivasa Rao Bonta
Postdoctoral Research Associate

Ph.D. in Materials Science and Engineering from National Institute for Materials Science. Japan

Research Interests
Development of novel metallic materials with improved structural and functional properties through severe plastic deformation by high pressure torsion; stabilization of high pressure phases in pure Zr and pure Ti by the application of shear under pressure.

Dr. Federico Sket
Postdoctoral Research Associate

Ph.D. in Materials Engineering from Max-Planck Institute for Iron Research. Germany

Research Interests
Development and application of state-of-the-art X-ray microtomography techniques to understand and characterize the deformation and damage mechanisms of advanced structural materials.

research assistants

Alexandros Charalambides

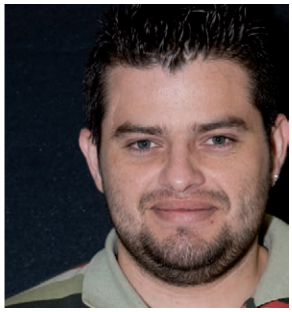
M.Eng.: University of Maryland Baltimore County. USA
Research: Multiscale Materials Modelling

Nathamar Dudamell

M.Eng.: Central University of Venezuela. Venezuela.
Research: Physical Metallurgy of Mg Alloys

Ana Fernández

M.Eng.: Carlos III University of Madrid. Spain
Research: Crystal Plasticity Modelling



Julián García

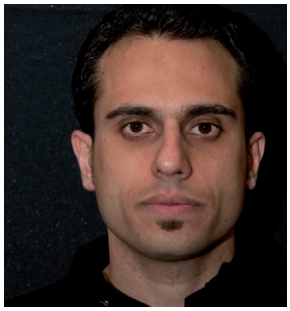
M.Eng.: Polytechnic University of Madrid. Spain
Research: Biological Cell Modelling

Deepak Hanumanthappa

M.Eng.: University of Stuttgart. Germany
Research: Numerical Simulation of Composites Impact

Silvia Hernández

M.Sc.: Complutense University of Madrid. Spain
Research: Processing of Composite Materials



Mohammad Ali Jabbari

M.Eng.: Isfahan University of Technology. Iran
Research: Solid State Processing of Metallic Alloys

Saeid Lotfian

M.Eng.: Isfahan University of Technology. Iran
Research: High Temperature Nanoindentation

Steven E. McHugh

M.Eng.: Tufts University. USA
Research: Biological Cell Modelling

Eva Cristina Moreno

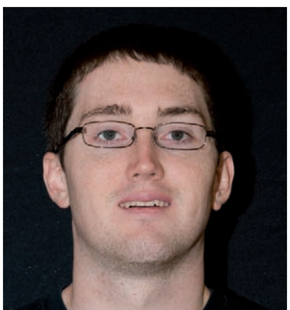
M.Eng.: University of Castilla la Mancha. Spain
Research: Mechanical Behaviour of Nanostructured Metals

Francisca Martínez

MEng: Carlos III University of Madrid. Spain
Research: Numerical Simulation of Composites under Impact

Rocío Muñoz

M.Eng.: Complutense University of Madrid. Spain
Research: Ti-Al Intermetallic Alloys



Raúl Muñoz

M.Eng.: Carlos III University of Madrid. Spain
Research: Computational Mechanics of Composite Materials

Nithin Palavalli

M.Eng.: Asia University. Taiwan ROC
Research: Atomistic Materials Modelling

Mehdi Rahimian

M.Eng.: Malek Ashtar University of Technology. Iran
Research: Solidification of Ni-based Superalloys

Marcos Rodríguez

M.Eng.: Complutense University of Madrid. Spain
Research: Micromechanics of Composites

Sergio Sádaba

M.Eng.: Public University of Navarre. Spain
Research: Virtual Testing of Composites

Rafael Soler

M.Eng.: Cranfield University. UK
Research: Nanomechanics

Joaquim Vilà

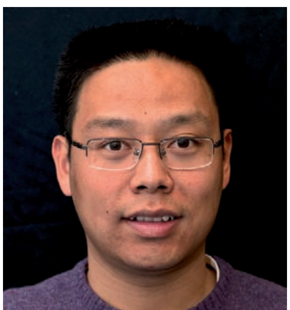
M.Eng.: University of Girona. Spain
Research: Processing of Composites by Infiltration

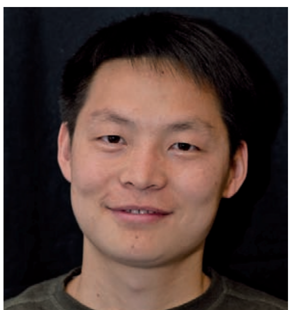
Guanglong Xu

M.Eng.: Central South University. China
Research: Computational Alloy Design

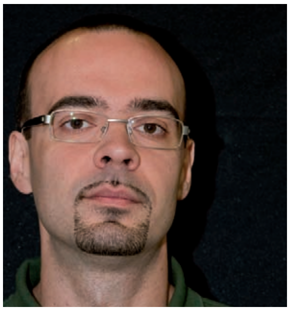
Hangbo Yue

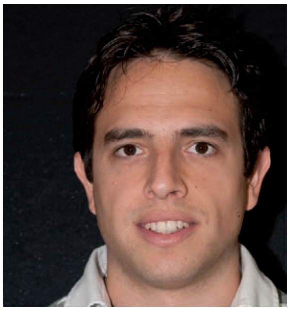
M.Eng.: Zhongkai University of Agriculture and Engineering. China
Research: Ecofriendly Polymer Nanocomposites





laboratory technicians



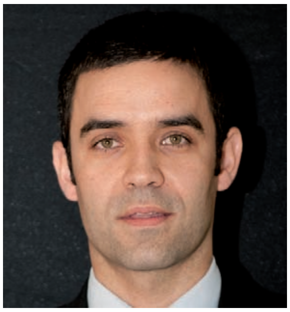


José Luis Jiménez
V.T.: Specialist Technician. Spain

Vanesa Martínez
M.Eng.: University of Valencia. Spain

Juan Carlos Rubalcaba
B.Eng.: Alcalá de Henares University. Spain

management and administration


Dr. Covadonga Rosado
Manager

Miguel Ángel Rodiel
Technology Manager

Vanessa Fernández
Personnel Manager

Eduardo Ciudad-Real
Accountant Responsible

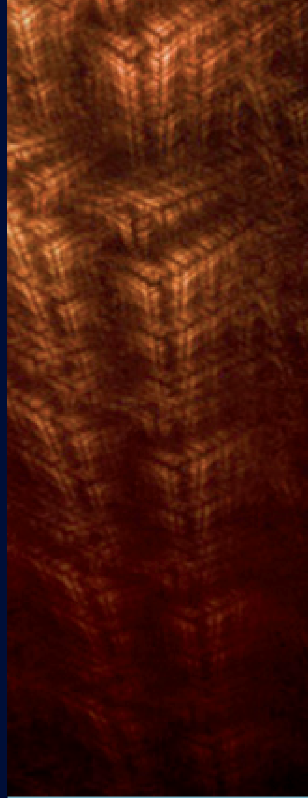
Borja Casilda
Accountant Assistant Trainee

Mariana Huerta
Secretary



5

scientific infrastructures



Current scientific infrastructures of IMDEA Materials Institute are located at the two provisional laboratories and they are detailed below.

5.1. Processing

- **Triple Roller Mill** (Exakt 80 E, Exact Technologies) to disperse fillers and additives in viscous matrix. The shearing forces to break agglomerate are generated by three hardcrome-plated rollers that rotate at different angular velocities and where gap (minimum 5 μm) and speed setting are controlled electronically. The machine is equipped with a cooling-heating unit which allows the temperature control on roller surface in a range of -10 – 100ºC.

- **Pultrusion Line** to manufacture continuous composite profiles of thermoset matrices reinforced with carbon, glass, aramid, and other advanced fibres. Fibre 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, Dynamic Systems Inc.) 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 Characterization

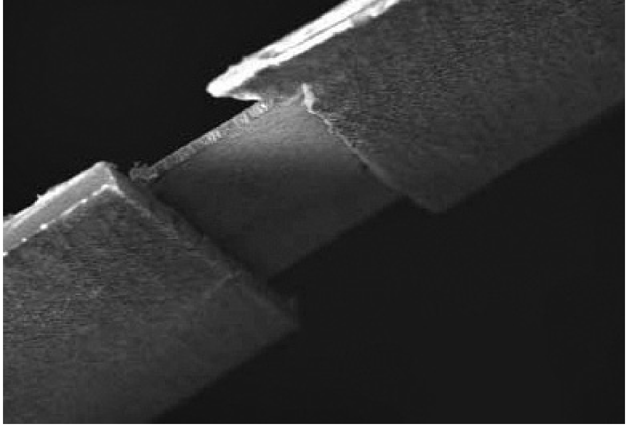
- **Atomic Force Microscope** (Park XE150, Park Systems) to carry out nanoscale characterization of materials, including non-contact and contact atomic force microscopy. Additional features include magnetic microscopy, thermal microscopy, nanolithography and a high temperature stage to carry out measurements up to 250ºC.

- **Scanning Electron Microscope** (EVO MA15, Zeiss) with chemical microanalysis (EDS Oxford INCA 350**)** and automated pressure regulation from 10 to 400 Pa to work with non-metallic samples without the need of metalizing.

- **Metallography Laboratory** to prepare samples for microstructural analysis. 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).

- IMDEA Materials Institute has signed an agreement with the Transmission Electron Microscopy Laboratory (LABMET) of the Physics Department at the Carlos III University for using the services of a **Field-Emission Scanning Transmission Electron Microscope** (FEG-STEM) equipped with digital camera, high-angle annular dark field (HAADF) and Energy Dispersive X-Ray Spectroscopy (EDS).

5.3. Mechanical Characterization

- **Dynamic Mechanical Analysis** (Q800, TA Instruments) to determine the elastic-viscous behaviour of materials, mainly polymers. The machine works in the temperature range of -150 – 600ºC, frequency range of 0.01 – 200 Hz and the maximum force is 18 N. Clamps for dual/single cantilever, 3 point bend, and tension are available.

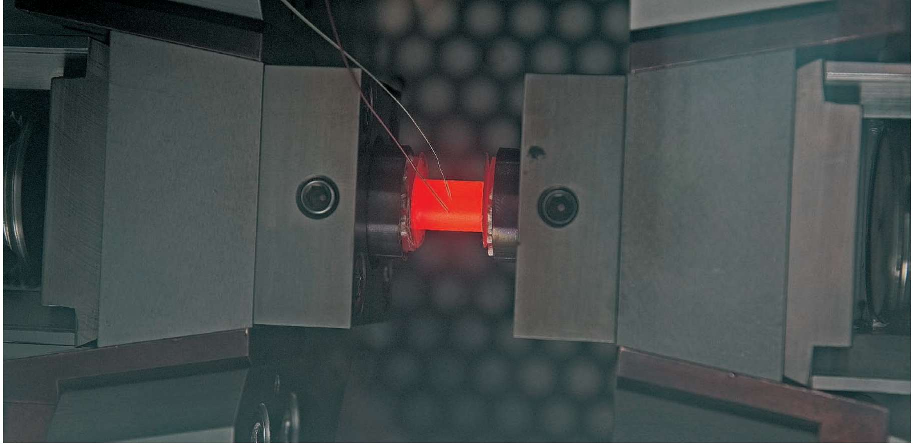
- **Digital Image Correlation System** (Vic-3D, Correlated Solutions) to perform non-contact full-field displacement mapping by means of images acquired by an optical system of stereographic cameras. The images obtained are compared to images in the reference configuration and used by the expert system to obtain the full 3D displacement field and the corresponding strains.

- **Nanoindentation System** (TI950, Hysitron) to perform instrumented nanoindentation, as well as other nanomechanical testing studies, such as micropillar compression in a range of materials, including test at temperatures up to 500ºC. The capabilities include nanoindentation with several loading heads tailored for different applications (maximum load resolution, 1 nN), dynamic measurements, scratch and wear testing and SPM imaging and modulus mapping performed with the same indenter tip.

- **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 for tension/compression and fibre tensile testing are available, with maximum loads of 10 kN and 1 N, respectively.

- **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.



5.4. Thermal Characterization

- **Dual Cone Calorimeter** (Fire Testing Technology) to study the forced combustion behaviour of polymers simulating real fire conditions; fire relevant properties including time-to-ignition, critical ignition flux heat release rates (HRRs), peak of HRR, mass loss rates (MLRs), smoke production, CO_2 and CO yields, effective heat of combustion, and specific extinction areas are directly measured according to ASTM/ISO standards.

- **UL94 Horizontal/Vertical Flame Chamber** (Fire Testing Technology), a widely used flame testing methodology, for selecting materials to be used as enclosures for electronic equipment and other consumer applications. Tests performed include horizontal burning test (UL94 HB), vertical burning test (UL94 V-0, V-1, or V-2), vertical burning test (5VA or 5VB), thin material vertical burning test (VTM-0, VTM-1 or VTM-2), and horizontal burning foamed material test (HF-1, HF-2 or HBF).

- **(Limiting) Oxygen Index** (Fire Testing Technology) to measure the relative flammability of a material by evaluating the minimum concentration of oxygen in precisely controlled oxygen-nitrogen mixture that will just support flaming combustion of a specimen.

- **Differential Scanning Calorimeter** (Q200, TA Instruments) to analyze thermal properties/phase transitions of different materials up to 725ºC. Equipped with Tzero technology, it provides highly reproducible baselines, superior sensitivity and resolution. It is also coupled with a refrigerated cooling system to operate over a temperature range of - 40 to 400ºC and higher cooling rates of ~50ºC/min.

- **Thermogravimetric Analyzer** (Q50, TA Instruments) to understand a materials' thermal stability and composition up to 1000ºC by analyzing the weight changes in a material at higher resolution as a function of temperature (or time) in a controlled atmosphere.

- **High Temperature Furnace** (Nabertherm, RHTH 120/600/16) to carry out heat treatments of up to temperatures of 1600ºC in vacuum or in an inert atmosphere.

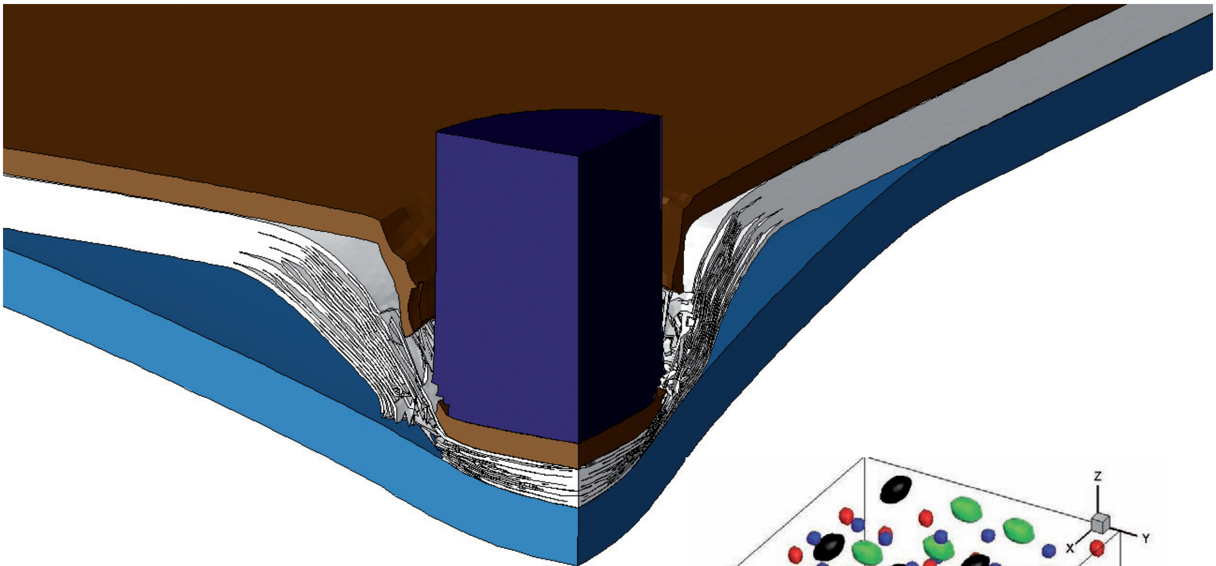
5.5. Simulation

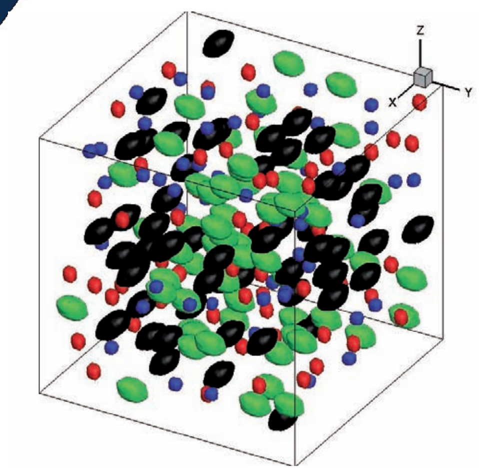
- **High Performance Computing Cluster** (108 cores, AMD Opteron 2356, 2431 & 6238).

- **High Performance Computing Servers** (8 cores AMD Opteron 8222SE, 8 cores INTEL Xeon X5450).

- Access to CeSViMa (Madrid Centre for Supercomputing and Visualization) and Mare Nostrum (Barcelona Supercomputing Centre) supercomputing facilities.

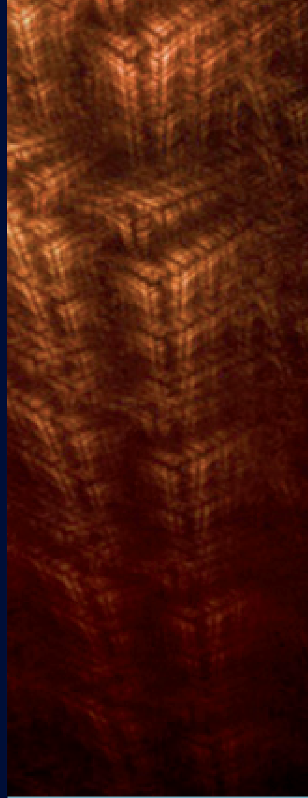
- Standard simulation, preprocessing and postprocessing programs (CALPHAD, DICTRA, Abaqus, Hypermesh, Tecplot, etc.) as well as in-house developed codes for modelling and simulation of the thermodynamic properties, phase-diagrams, mechanical behaviour and damage evolution of engineering materials.





6

research projects



IMDEA Materials Institute currently participates in 35 research projects, 15 of which began in 2011, leading to a 47% increase in the competitive and industrial funds attracted by the institute with respect to 2010. As shown in Figure 5, the project portfolio is divided into three main groups: 14 projects were obtained in international competitive calls, out of which 13 are funded by the European Union and 1 is jointly supported by the National Science Foundation of the US and the Spanish Ministry of Economy and Innovation (MEI) within the Materials World Network Programme. 8 projects are funded by national programs sponsored by MEI and the Regional Government of Madrid, and finally 13 Industrial contracts, several of which are supported by the Spanish Centre for Technological and Industrial Development (CDTI).

Figure 5. Active research projects by funding source

A brief description of several projects started in 2011 is provided below:

GOBIERNO DE ESPAÑA MINISTERIO DE CIENCIA E INNOVACIÓN

trainer

acciona Infraestructuras

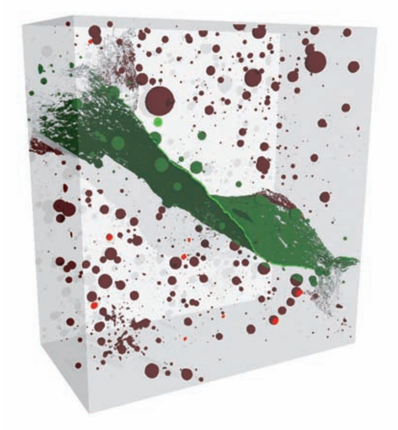
TRAINER

"Smart and self healing technology of materials"

Funding: **Centre for Industrial Technological Development (CENIT Programme), Spanish Ministry of Science and Innovation**
Partners: National consortium led by Acciona Infraestructuras, IMDEA Materials Institute collaborates with Acciona Infraestructuras
Duration: **2011-2013**
Principal Investigator: **Dr. F. Sket**

The CENIT project TRAINER (Smart Self Healing Technology of Materials) is aimed at developing the knowledge and technology necessary to obtain materials that repair autonomously and automatically without human intervention after suffering damage, recovering their initial aesthetic and mechanical properties. The project is led by ACCIONA Infraestructuras and involves another 12 companies and 21 research centres and universities.

Self-healing is a very attractive concept to enhance the durability and reliability of materials in structural applications and it has been screened in different systems using



different strategies. Among them, self-healing polymer systems which contain a liquid healing agent stored in microcapsules are a very prominent example. The objective of IMDEA Materials Institute activities in the project is to study the process of self-healing in these polymer systems by means of X-ray computer-assisted nanotomography. The investigation involves the observation of the actual release process of the healing agent from broken capsules near the crack tip and the posterior process of healing.

MASTIC

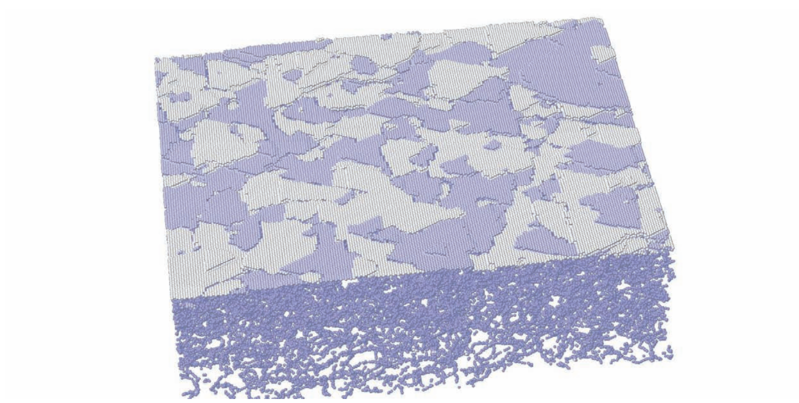
"Multi atomistic Monte Carlo simulation of technologically important crystals"

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**
Duration: **2011-2015**
Principal Investigator: **Dr. I. Martin-Bragado**

SEVENTH FRAMEWORK PROGRAMME

COFUNDED BY MARIE CURIE ACTIONS

This European project is aimed at the development and application of atomistic Object and Lattice Kinetic Monte Carlo techniques (OKMC, LKMC) tools to improve the scientific understanding and provide a simulation workbench to optimize the use of SiGe and SiC in microelectronics and of Fe and FeCr in nuclear applications. In particular, LKMC will be used to study the amorphous/crystalline transitions and the formation of defects during these transitions in Si-based materials. In addition, models for the inclusion of binary alloys in an OKMC scenario will be created to study the evolution of defects in SiC, SiGe and FeCr materials under different conditions. Finally, parallelization techniques will be explored to improve the scope of KMC applications. The knowledge gain with this project will improve the performance of the last generation Si-based transistors and enhance the application of FeCr as a blanket material in the ITER and DEMO projects as well as in other fusion reactor concepts.



RADINTERFACES

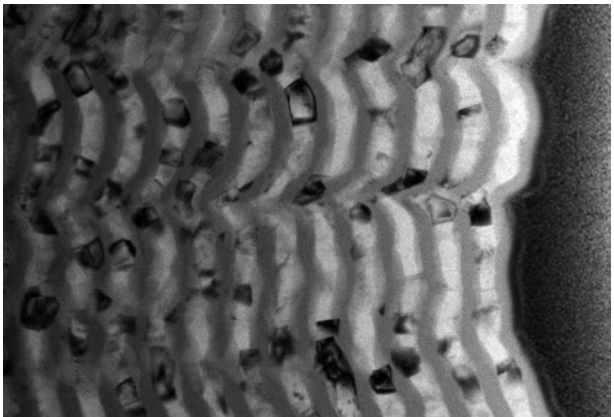
"Multiscale modelling and materials by design of interface-controlled radiation damage in crystalline materials"

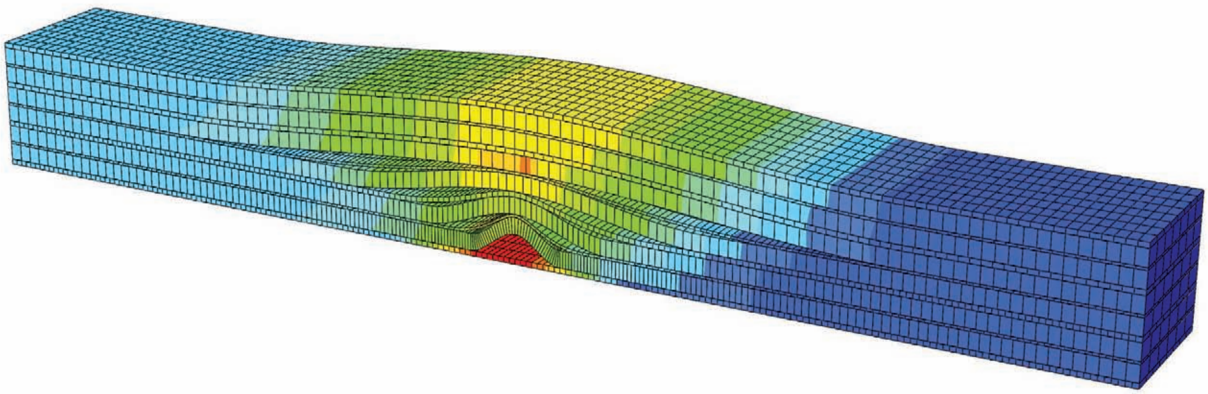
SEVENTH FRAMEWORK PROGRAMME

Funding: **NMP, European Union-7th Framework Programme**
Partners: Centre National de la Recherche Scientifique (France), University of Oviedo (Spain), University of Burgos (Spain), Ecole des Mines de Paris (France), Czech Technical University of Prague (Czech Republic), Universita degli Studi di Cagliari (Italy), University of Tartu (Estonia), Uppsala University (Sweden) and IMDEA Materials Institute (Spain).
Duration: **2011-2014**
Principal Investigator: **Prof. J. LLorca**

Radiation damage is known to lead to materials failure and thus is of critical importance to lifetime and safety within nuclear reactors. While materials mechanical behaviour under irradiation has been subject to numerous studies, the current predictive capabilities appear limited. Observations and physical models have shown that the most important damage contributions arise from point defect localization –leading to void swelling- and creep. It was recently found that void swelling can be prevented via the use of nanoscale metallic multilayers with non coherent heterophase interfaces. Unfortunately, no tool is available to generally predict the effect of interface composition (monophase, heterophase) and structure (geometry, roughness) on its propensity to resist radiation damage (both via defect localization and creep). These limitations motivate the proposed study which aims at developing such tool. Given the multi-scale multi physics nature of the problem, the consortium is formed by experts in the fields of materials modelling via *ab initio*, molecular dynamics and continuum modelling as well as of materials characterization and processing via mechanical alloying and physical vapour deposition.

The program aims at constructing a bottom-up framework allowing discovery and quantifications of materials damage mechanisms and effects on mechanical properties for novel crystalline materials with large interfacial areas. Model validation will arise through direct comparison with materials testing for a wide array of materials systems (metal/metal, metal/oxide, oxide/oxide). The main tasks of IMDEA Materials Institute are the development of the multiscale modelling tools based on Kinetic Monte Carlo, dislocation dynamic and crystal plasticity, and the mechanical characterization of the materials via nano-micromechanical testing.





AZIMUT

"Offshore wind energy 2020"

Funding: **Centre for Industrial Technological Development (CENIT Programme), Spanish Ministry of Science and Innovation**
Partners: National consortium led by Gamesa, IMDEA Materials Institute collaborates with Gamesa
Duration: **2011-2013**
Principal Investigators: **Dr. C. González and Dr. C. S. Lopes**

GOBIERNO DE ESPAÑA MINISTERIO DE CIENCIA E INNOVACIÓN

Gamesa

The CENIT project AZIMUT is aimed at generating the know-how required to develop a large-scale marine wind turbine using 100 percent Spanish technology. This includes overcoming the challenges of constructing offshore wind turbine foundations, energy delivery to land, and narrowing the gap between the cost of offshore and onshore wind energy sites. If these hurdles can be overcome, the plan is to construct a large-scale offshore wind turbine with a capacity of 15 MW by 2020. The project is coordinated by Gamesa and includes another 10 companies as well as 22 universities and research centres.

The main objective of the collaboration between Gamesa and IMDEA Materials Institute is to apply advanced simulation tools to predict the mechanical behaviour of composite materials for wind turbine blades in order to improve offshore reliability, including the analysis of the effect of defects. Different types of manufacturing defects (fabric wrinkles, voids, ply cutting, thickness variation, etc.) will be studied by means of state-of-the-art virtual test methodology developed by IMDEA Materials Institute.

NewQP

“New advanced high strength steels by the quenching and partitioning process”

Funding: **Research Fund for Coal & Steel, European Union-7th Framework Programme**
Partners: Fundació CTM Centre Tecnològic (Coordinator, Spain), ThyssenKrupp Steel Europe AG (Germany), Arcelor-Mittal (Belgium), Centro Sviluppo Materiali (Itlay), IMDEA Materials Institute (Spain), University of Gent (Belgium) and Delft University of Technology (The Netherlands).
Duration: **2011-2014**
Principal Investigator: **Dr. I. Sabirov**

This EU-funded project aims at developing new advanced high strength steel grades for automotive applications by means of the Quenching and Partitioning (Q&P) process. Q&P opens the way to develop steel microstructures based on the exceptionally advantageous combination of austenitic and martensitic phases at the industrial scale, leading to materials with improved strength, ductility and strain hardening capability. The industrial applicability of the Q&P process will be improved in terms of compositions, treatments and properties as galvanisability and weldability to develop a controlled and reproducible production process for these materials, and to be ready for future developments.

IMDEA Materials Institute will study the deformation and fracture behaviour of the Q&P steels at the macro-, micro-, and nano-scales using state-of-the-art characterization techniques. This information will provide a fundamental understanding of the microstructure-properties relationship, which will lead to further improvement of the mechanical properties. IMDEA Materials Institute will also develop a theoretical Ginzburg-Landau model to describe the formation of a mixed microstructure that is governed by the interplay and competition between various microstructural transformations.

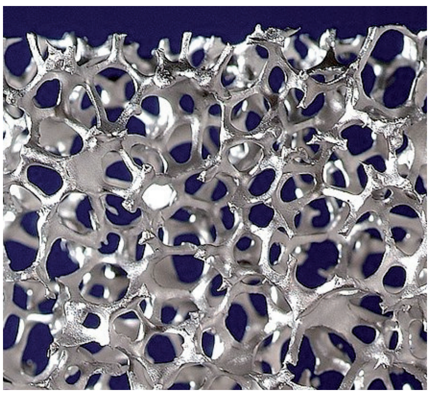
VINAT

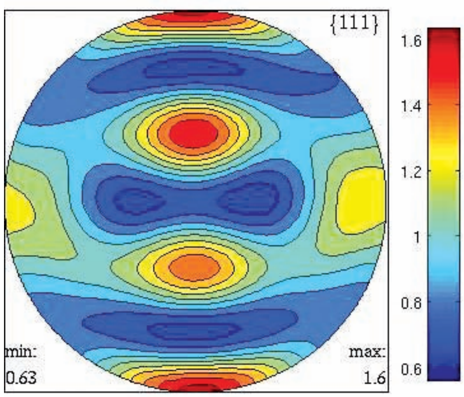
"Theoretical analysis, design and virtual testing of biocompatibility and mechanical properties of Titanium-based nanomaterials"

Funding: **NMP, European Union-7th Framework Programme (Coordinated call with Russia)**
EU Partners: Technical University of Denmark (Denmark), IMDEA Materials Institute (Spain), Katholieke Universiteit Leuven (Belgium), Goethe University Frankfurt am Main (Germany), Technion (Israel) and Timplant Ltd. (Czech Republic).
Russian Partners: National University of Science and Technology (Moscow), Ufa State Aviation Technical University (Ufa), Institute of Strength Physics and Materials Science (Tomsk), Scientific-Industrial Enterprise "Metal" (Moscow), NanoMeT Ltd. (Ufa).
Duration: **2011-2014**
Principal Investigators: **Dr. I. Sabirov**

This project is devoted to the development of multiscale models for the theoretical analysis, virtual testing and optimization of three main groups of nanostructured titanium-based metallic materials: pure titanium, Ti-Nb alloy and superelastic/shape memory Ti-Ni alloy. The idea of the project is to develop and validate a series of computational models for these materials at the atomistic, crystal/dislocation and grain/texture/microstructure levels, to explore their biocompatibility and mechanical properties, and to analyse the effect of atomistic, nano and microscale structures on the properties of these materials. Models based on the methods of molecular dynamics, dislocation dynamics, single crystal plasticity, polycrystal homogenization, discrete micromechanics are employed here to analyze the mechanical properties and biocompatibility of Ti-based nanomaterials.

The IMDEA Materials team will contribute to the project in three different areas: modelling and simulation of nanostructured Ti by means of molecular dynamics, dislocation dynamics and crystal plasticity models; experimental characterization of the actual deformation mechanisms; and validation of the modelling results.



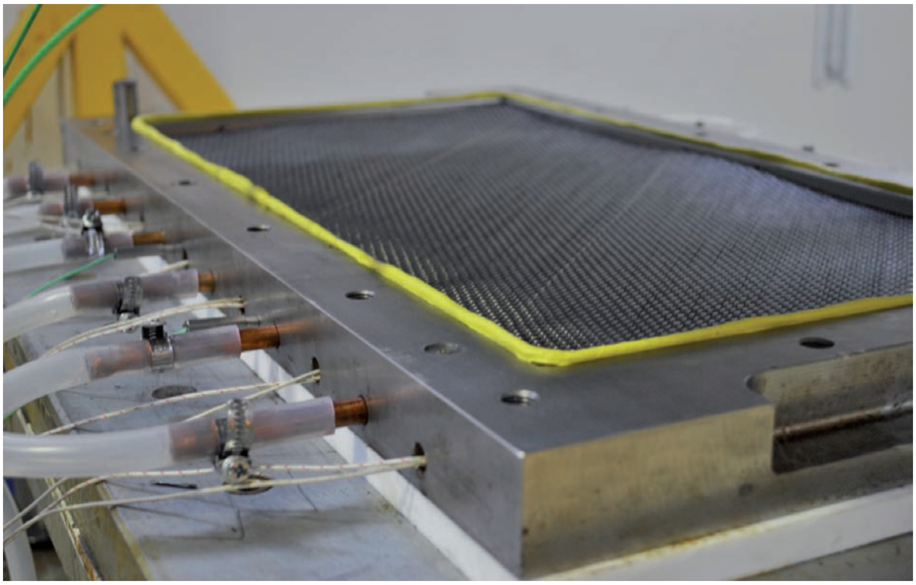


SEMICURED

“Semi-cured products manufacturing”

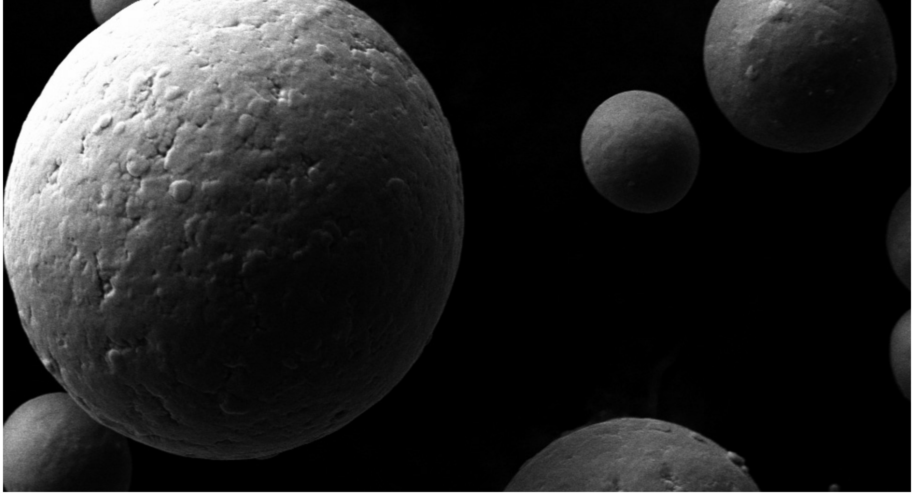
Funding: **Airbus Operations S.L.**
Duration: **2011-2012**
Principal Investigators: **Dr. C. González**

This project aims to develop new processing routes for manufacturing partially-cured composite parts by means of resin transfer moulding. These parts will be able to be post-cured and consolidated with traditional prepregs counterparts. The results of the project will provide important knowledge for manufacturing one-shot integrated composite parts, leading to shorter production times and lower cost.



MAGMAN (“Analysis of the microstructural evolution and mechanical behaviour of Mg-Mn-rare earth alloys”)

Funding: **Spanish Ministry of Economy and Competitiveness-National Science Foundation, USA (Materials World Network Program)**
Partners: IMDEA Materials Institute, Polytechnic University of Madrid and Michigan State University (USA).
Duration: **2011-2014**
Principal Investigators: **Dr. M.T. Pérez-Prado**



ASKME ("Atomistic silicon kinetic Monte Carlo modelling for microelectronics")
Funding: **Synopsys Inc. (USA)**
Duration: **2011-2013**
Principal Investigators: **Dr. I. Martin-Bragado**

SIMET ("Numerical simulations for metallic fragments impact on composites solutions"
Funding: **Airbus Operations S.L.**
Duration: **2011-2012**
Principal Investigator: **Dr. C. González**

MASID ("Modelling of advanced semiconductor integrated devices")
Funding: **Global Foundries Singapore Pte Ltd. (Singapore)**
Duration: **2011-2014**
Principal Investigator: **Dr. I. Martin-Bragado**

CAREFIB ("Development of carbon nanotube-based epoxy resins for high performance fibre cables")
Funding: **Centre for Industrial Technological Development (CDTI)**
Duration: **2011-2012**
Principal Investigator: **Dr. J. J. Vilatela**

VIRTEC ("Virtual testing of low-velocity impact on carbon fibre composites")
Funding: **Airbus Operations S. L.**
Duration: **2011-2012**
Principal Investigators: **Dr. C. S. Lopes**

DECOMP ("Development of advanced ecofriendly polymer nanocomposites with multifunctional properties")

Funding: **Chinese Scholarship Council (China)**

Duration: **2011-2014**

Principal Investigators: **Dr. J. J. Vilatela & Prof. J. LLorca**

MODELQP ("Ginzburg-Landau model for the mixed microstructure in new Q&P steels")

Funding: **Chinese Scholarship Council (China)**

Duration: **2011-2014**

Principal Investigators: **Dr. Y. Cui & Prof. J. LLorca**

Other research projects currently running at IMDEA Materials Institute are:

IMS & CPS ("Innovative material synergies & composite processing strategies")

Funding: **NMP, European Union-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**

ICE SHEDDING ("Design of advanced shields against high-velocity ice impact")

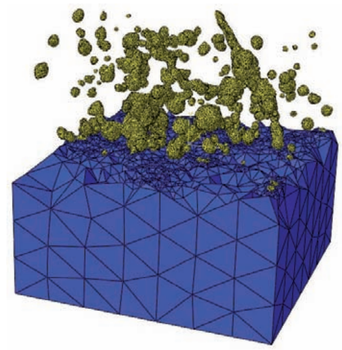
Funding: **Airbus Operations**

Duration: **2010-2012**

Principal Investigator: **Dr. C. González**

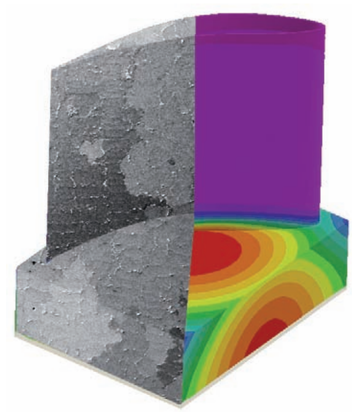
ALTIVA ("Development of advanced gamma TiAl alloys for components with high reliability: microstructure design and modelling of the mechanical behaviour")

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



CAJAL BLUE BRAIN

Funding: **Spanish Ministry of Science and Innovation**
Partners: Polytechnic University of Madrid, Biomedical Research Institute of Barcelona-CSIC, Ramón y Cajal Hospital, Carlos Haya Hospital, Cajal Institute-CSIC, Rey Juan Carlos University, Castilla la Mancha University and IMDEA Materials Institute
Duration: **2010-2013**
Principal Investigator: **Dr. A. Jérusalem**



VANCAST ("Next generation nozzle guide vanes")

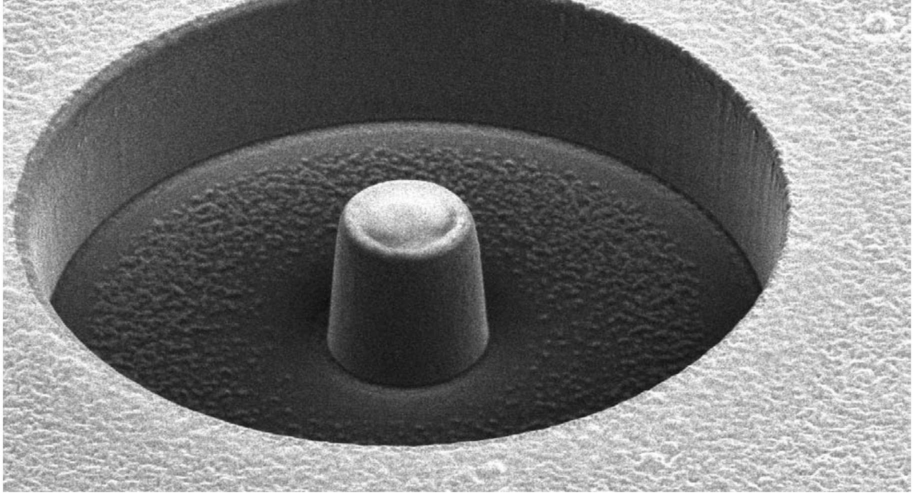
Funding: **ERA-Matera+, European Union-7th Framework Programme**
Partners: IMDEA Materials Institute (coordinator), Industria de Turbo Propulsores (ITP), Precicast Bilbao, Calcom-ESI, University of Applied Sciences of Switwerland and Precicast Novazzano
Duration: **2010-2013**
Principal Investigators: **Prof. J. LLorca and Dr. I. Sabirov**

SIMUCOMP ("Advanced numerical simulations of inter- and intralaminar failures in composite")

Funding: **ERA-Matera+, European Union-7th Framework Programme**
Partners: IMDEA Materials Institute (coordinator), Université de Liège, CENAERO, Centre de Recherche Public Henri Tudor and e-Xstream Engineering
Duration: **2010-2013**
Principal Investigator: **Dr. A. Jérusalem**

ELSITEG "Electrospinning of silk fibroin solutions for tissue engineering"

Funding: **Polytechnic University of Madrid and IMDEA Materials Institute**
Partners: Polytechnic University of Madrid (Biologic Materials and Biomaterials Research Group) and IMDEA Materials Institute
Duration: **2010-2012**
Principal Investigators: **Prof. J. LLorca & Dr. A. Dasari**



HOTNANO (“High temperature nanoindentation”)

Funding: **Altare S. L.**

Duration: **2010-2013**

Principal Investigator: **Dr. J. M. Molina-Aldareguía**

ESTRUMAT (“Advanced structural materials”)

Funding: **Regional Government of Madrid, General Direction for Research**

Partners: Rey Juan Carlos University (coordinator), IMDEA Materials Institute, 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: **Centre for Industrial Technological Development (CENIT Programme), Spanish Ministry of Science and Innovation**

Partners: National consortium led by Boeing Research, IMDEA Materials Institute collaborates with Aernnova Engineering Solutions Ibérica and Aries Complex Aeronáutica

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), IMDEA Materials Institute, Swerea-Sicomp and APC-Composite

Duration: **2010-2012**

Principal Investigator: **Dr. A. Jérusalem**

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

Funding: **Spanish Ministry of Science and Innovation (Fundamental Research Programme)**
Partners: IMDEA Materials Institute and 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: IMDEA Materials Institute and 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**

DEFCOM ("The effect of defects in structural composites")

Funding: **ERA-Net MATERA, European Union-6th Framework Programme,**
Partners: IMDEA Materials Institute (coordinator), 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: **ERA-Net MATERA, European Union-6th Framework Programme,**

Partners: Tyndall National Institute (coordinator), IMDEA Materials Institute, Dublin City University and the Institute of Materials Science of Madrid (CSIC)

Duration: **2009-2011**

Principal Investigator: **Dr. J. M. Molina-Aldareguía**

ICARO (“Advanced composites innovation and rear end optimization”)

Funding: **Centre for Industrial Technological Development (CENIT Programme), Spanish Ministry of Science and Innovation**

Partners: National consortium led by Airbus, IMDEA Materials Institute collaborates with Aries Estructuras Aeroespaciales and Airbus Military

Duration: **2009-2011**

Principal Investigator: **Dr. C. González**

MAAXIMUS (“More affordable aircraft structure lifecycle through extended, integrated, & mature numerical sizing”)

Funding**: Transport, European Union-7th Framework Programme**

Partners: Consortium of 58 European partners from 18 countries led by Airbus

Duration: **2008-2012**

Principal Investigator: **Prof. J. LLorca**

FUTURE PBO (“Analysis and optimization of PBO cables under service conditions”)

Funding**: Spanish Ministry of Science and Innovation (TRACE Programme) and Future Fibres S.L.U.**

Partners: IMDEA Materials Institute (coordinator) and Future Fibres S.L.U.

Duration: **2008-2011**

Principal Investigator: **Dr. C. González**

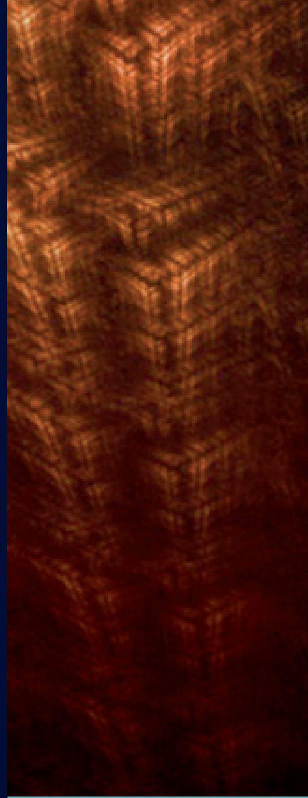
MAGNO (“Magnesium new technological opportunities”)

Funding**: Centre for Industrial Technological Development (CENIT Programme), Spanish Ministry of Science and Innovation**

Partners: National consortium led by Grupo Antolin, IMDEA Materials Institute collaborates with Grupo Antolin

Duration: **2008-2011**

Principal Investigator: **Dr. M. T. Pérez-Prado**



7 dissemination results

publications

7.1. Publications

1. N. V. Dudamell, I. Ulacia, F. Gálvez, S. Yi, J. Bohlen, D. Letzig, I. Hurtado, M. T. Pérez Prado. *"Twinning and grain subdivision during dynamic deformation of a Mg AZ31 sheet alloy at room temperature"*. **Acta Materialia, 59**, 6949-6962, 2011.

2. K. Dzieciol, A. Borbély, F. Sket, A. Isaac, M. di Michiel, P. Clotens, T. Buslaps, A. R. Pyzalla. *"Void growth in copper during high-temperature power-law creep"*. **Acta Materialia 59**, 671-677, 2011.

3. J. LLorca, C. González, J. M. Molina-Aldareguía, J. Segurado, R. Seltzer, F. Sket, M. Rodríguez, S. Sádaba, R. Muñoz, L. P. Canal. *"Multiscale modeling of composite materials: a roadmap towards virtual testing"*. **Advanced Materials 23**, 5130-5147, 2011.

4. Martin-Bragado, V. Moroz. "*Modeling of {311} facets using a lattice kinetic Monte Carlo three-dimensional model for selective epitaxial growth of silicon"*. **Applied Physics Letters, 98,** 153111, 2011.

5. Martin-Bragado. *"{111} local configurations: The main source of silicon defects during solid phase epitaxial regrowth modeled by lattice kinetic Monte Carlo"*. **Applied Physics Letters, 98,** 233109, 2011.

6. W. B. Li, Y. -W. Cui, R. Hu, H. Zhong, H. Chang, J. S. Li, L. Zhou. *"Assessment of atomic mobility for the bcc phase of the Ti-Al-Cr system"*. **CALPHAD 35**, 384–390, 2011.

7. I. Montealegre Melendez, E. Neubauer, P. Angerer, H. Danninger, J. M. Torralba. *"Influence of nano-reinforcements on the mechanical properties and microstructure of titanium matrix composites"*. **Composites Science and Technology 71**, 1154–1162, 2011.

8. S. Hernández, F. Sket, J. M. Molina-Aldareguía, C. González, J. LLorca. *"Effect of curing cycle on void distribution and interlaminar shear strength in polymer-matrix composites"*. **Composites Science and Technology 71**, 1331–1341, 2011.

9. T. A. Sebaey, N. Blanco, C. S. Lopes, J. Costa. *"Numerical investigation to prevent crack jumping in Double Cantilever Beam tests of multidirectional composite laminates"*. **Composites Science and Technology 71**, 1587-1592, 2011.

10. T. A. Sebaey, C. S. Lopes, N. Blanco, J. Costa. *"Ant Colony Optimization for Dispersed Laminated Composite Panels under Biaxial Loading"*. **Composite Structures 94**, 31–36, 2011.

11. M. Agoras, P. Ponte Castañeda. *"Homogenization estimates for multi-scale nonlinear composites"*. **European Journal of Mechanics. A/Solids 30**, 828-843, 2011.

12. S. Milenkovic, A. Schneider, G. Frommeyer. *"Constitutional and microstructural investigation of the pseudobinary NiAl-W system"*. **Intermetallics 19**, 342-349, 2011.

13. S. Malekjani, P. D. Hodgson, P. Cizek, I. Sabirov, T. B. Hilditch. *"Cyclic deformation response of UFG 2024 Al alloy*". **International Journal of Fatigue 33**, 700-709, 2011.

14. R. Seltzer, A. P. Cisilino, P. M. Frontini, Y. Mai. *"Determination of the Drucker–Prager parameters of polymers exhibiting pressure-sensitive plastic behaviour by depth-sensing indentation"*. **International Journal of Mechanical Sciences 53**, 471-478, 2011.

15. A. Fernández, M. T. Pérez-Prado, Y. Wei, A. Jérusalem. *"Continuum modeling of the response of a Mg alloy AZ31 rolled sheet during uniaxial deformation"*. **International Journal of Plasticity 27**, 1739-1757, 2011.

16. A. Ridruejo, C. González, J. LLorca. *"Micromechanisms of deformation and fracture of polypropylene nonwoven fabrics*". **International Journal of Solids and Structures 48**, 153-162, 2011.

17. M. C. Mesa, P. B. Oliete, V. M. Orera, J. Y. Pastor, A. Martín, J. LLorca. *"Microstructure and mechanical properties of* $Al_2O_3/Er_3Al_5O_{12}$ *eutectic rods grown by the laser-heated floating zone method"*. **Journal of the European Ceramic Society 31**, 1241-1250, 2011.

18. J. Sicre-Artalejo, M. Campos, J. M. Molina-Aldareguía, J. M. Torralba. *"Quantification of hardening in Fe–Mn master alloys prepared by a mechanical alloying process via nanoindentation experiments"*. **Journal of Materials Research 26**, 1726 – 1733, 2011.

19. P. Ponte Castañeda, E. Galipeau. *"Homogenization-based constitutive models for magnetorheological elastomers at finite strain*". **Journal of the Mechanics and Physics of Solids 59**, 194-215, 2011.

20. A. Borbély, K. Dzieciol, F. Sket, A. Isaac, M. di Michiel, T. Buslaps, A.R. Pyzalla. "*Characterization of Creep and Creep Damage by In-situ Microtomography"*. **JOM Journal of the Minerals, Metals and Materials Society 63**, 78-84, 2011.

21. M. V. Aguirre, A. Martín, J. Y. Pastor, J. LLorca, M. A. Monge, R. Pareja. *"Mechanical properties of tungsten alloys with Y2O3 and titanium additions"*. **Journal of Nuclear Materials 417**, 516-519, 2011.

22. E. C. Moreno-Valle, I. Sabirov, M. T. Perez-Prado, M. Yu. Murashkin, E. V. Bobruk, R. Z. Valiev. *"Effect of the grain refinement via SPD on strength properties and deformation behaviour of an Al6061 alloy at room and cryogenic temperatures"*. **Materials Letters 65**, 2917-2919, 2011.

23. A. P. Zhilyaev, I. Sabirov, G. González-Doncel, J. Molina-Aldareguía, B. Srinivasarao, M.T. Pérez-Prado. *"Effect of Nb additions on the microstructure, thermal stability and mechanical behavior of high pressure Zr phases under ambient conditions"*. **Materials Science and Engineering 528**, 3496-3505, 2011.

24. J. Ballarre, R. Seltzer, E. Mendoza, J. C. Orellano, Y. Mai, C. García, S. M. Ceré. *"Morphologic and nanomechanical characterization of bone tissue growth around bioactive sol–gel coatings containing wollastonite particles applied on stainless steel implants"*. **Materials Science and Engineering C 31**, 545-552, 2011.

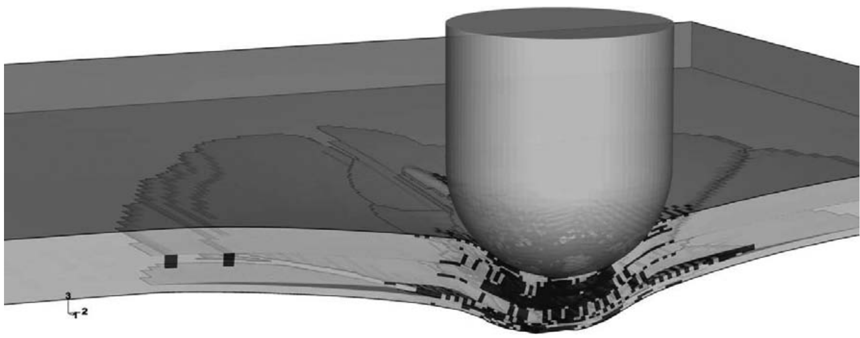
25. J. M Torralba, R. de Oro, M. Campos. *"From sintered iron to high performance PM steels"*. **Materials Science Forum 672**, 3-11, 2011.

26. A. Isaac, A. Borbély, K. Dzieciol, F. Sket, A. R. Pyzalla. *"In situ microtomographic characterization of single cavity-growth during high-temperature creep of leaded brass"*. **Metallurgical and Materials Transactions A 42**, 3022-3030, 2011.

27. R. Seltzer, F. M. de la Escalera, J. Segurado. *"Effect of water conditioning on the fracture behavior of PA12 composites processed by selective laser sintering"*. **Materials Science and Engineering A 528**, 6927-6933, 2011.

28. Z. Zuberova, I. Sabirov, Y. Estrin. *"The effect of deformation processing on tensile ductility of magnesium alloy AZ31"*. **Metallic Materials 49**, 29-36, 2011.

29. Y. -W. Cui, B. Tang, R. Kato, R. Kainuma, K. Ishida. *"Interdiffusion study of Co-Al binary alloys"*. **Metallurgical and Materials Transactions A 42**, 2542-2546, 2011.



30. J. M. Molina-Aldareguía, M. Rodríguez, C. González, J. LLorca. *"An experimental and numerical study of the influence of local effects on the application of the fibre push-in test"*. **Philosophical Magazine 91**, 1293-1307, 2011.

31. R. A. Lebensohn, M. I. Idiart, P. Ponte Castañeda, P.-G. Vincent. *"Dilatational viscoplasticity of polycrystalline solids with intergranular cavities"*. **Philosophical Magazine 91**, 3038-3067, 2011.

32. A. Jérusalem. "*Continuum modeling of the reverse Hall–Petch effect in nanocrystalline metals under uniaxial tension: how many grains in a finite element model?"*. **Philosophical Magazine Letters 91**, 599-609, 2011.

33. S. Milenkovic, S. Drensler, A. W Hassel. *"A novel concept for the preparation of alloy nanowires"*. **Physica Status Solidi A 208**, 1259-1264, 2011.

34. R. Seltzer, J. Kim, Y. Mai. *"Elevated temperature nanoindentation behaviour of polyamide 6"*. **Polymer International 60**, 1753-1761, 2011.

35. N. Lahellec, P. Ponte Castañeda, P. Suquet. *"Variational approximations for the effective response and filed statistics in thermoelastic composites with non-uniform phases"*. **Proceedings of the Royal Society of London A 467**, 2224-2246, 2011.

36. A. Jérusalem, A. Fernández, M. T. Pérez-Prado. *"Continuum modeling of {10-12} twinning in a Mg-3%Al-1%Zn rolled sheet"*. **Revista de Metalurgia 46**, 133-137, 2011.

37. B. Srinivasarao, A. P. Zhilyaev, M. T. Pérez-Prado. *"Orientation dependency of the alpha to omega+beta transformation in commercially pure zirconium by high pressure torsion"*. **Scripta Materialia 65**, 241-244, 2011.

38. I. Sabirov, M. T. Perez-Prado, J. M. Molina-Aldareguia, I. P. Semenova, G. K. Salimgareeva, R. Z. Valiev. *"Anisotropy of mechanical properties in high strength ultra-fine grained pure Ti processed via a complex severe plastic deformation route*". **Scripta Materialia 64**, 69-72, 2011.

7.2. Book Chapters

1. N. Ma, C. Shen, Y. -W. Cui, N. Zhou, Y. Wang. *"Coupling Microstructure Characterization with Microstructure Evolution"* in **Computational Methods for Microstructure-Property Relationships**, (S. Ghosh, D. Dimiduk, Eds.), Springer, MA, 151-197, 2011.

2. R. A. Lebensohn, P. Ponte Castañeda, R. Brenner, O. Castelnau. *"Full-field vs. homogenization methods to predict microstructure-property relationships of polycrystalline materials"*, in **Computational Methods for Microstructure-Property Relationships**, (S. Ghosh, D. Dimiduk, Eds.), Springer, MA, 393-441, 2011.

3. J. LLorca, C. González. *"Virtual mechanical testing of composites: from materials to components"* in **1st World Congress on Integrated Computational Materials Engineering**, (J. Allison, P. Collins and G. Spanos, eds.) TMS, Warrendale, PA, 121-127, 2011.

4. J. LLorca. *"Advances and challenges in the computational simulation of composites"*. **32nd Risø International Symposium on Materials Science** - Composite Materials for Structural Performance: Towards Higher Limits. (S. Faester, D. Juul Jensen, B. Ralph, B. F. Sørensen, Eds.), Risø DTU, Roskilde, Denmark, 45-57, 2011.

book chapters

7.3. Patents

1. *"Controlled fabrication of stable beta phase in the pure metals of group IV of the periodic table"*. A. P Zhilyaev, M. T. Pérez-Prado, A. Sharafutdinov. Patent ES2342962 (Spain).

2. *"Method to design a synthetic fibres cable"*. C. González, J. M. Molina, K. Tamargo, J. LLorca. Patent application P201031862 (Spain). Joint ownership with Future Fibres rigging systems S.L.

3. "*Process to improve the compression strength of PBO fibres and the PBO fibres obtained by this process"*. J. M. Molina-Aldareguia, K. Tamargo, C. González, J. LLorca, E. Lorenzo. Patent application P201001483 (Spain). Joint ownership with Future Fibres rigging systems S.L.

4. *"Method to obtain the beta phase of a transition pure metal of the group IV of the periodic system and product resulting from this method"*. M. T. Pérez-Prado, A. P Zhilyaev, A. Sharafutdinov. Patent application P200901060 (Spain) and PCT/ES2010/070017.

patents

7.4. International Congresses

7.4.1. Invited and Plenary Talks

1. *"Constitutive models for multi-scale, multi-physics material systems via nonlinear homogenization"*. P. Ponte Castañeda. **NSF Workshop on Challenges and Opportunities for Research in Multiscale Modeling in Mechanics of Materials**. Atlanta, USA, January 2011.

2. *"Functional Devices from Directionally Grown Nanowire Arrays"*. S. Milenkovic, A. W Hassel. **DFG Symposium on Nanowires and Nanotubes – from controlled Synthesis to Function**. Bonn, Germany, March 2011.

3. *"Constitutive response of porous elastomers*". P. Ponte Castañeda. **IUTAM Symposium on Mechanics of Liquid and Solid Foams**. Austin, USA, May 2011.

4. *"Virtual mechanical testing of composites: from materials to components"*. J. LLorca, C. González. **1st World Congress on Integrated Computational Materials Engineering**. Seven Springs, Pennsylvania, July, 2011.

5. *"Advances and challenges in the computational simulation of composites"*. J. LLorca. **32nd Risø International Symposium on Materials Science**: Composite Materials for Structural Performance: Towards Higher Limits. Røskilde, Denmark, September, 2011.

6. *"In-situ analysis of deformation and recrystallization mechanisms"*. M. T. Pérez-Prado, C. Boehlert, J. LLorca, I. Gutiérrez-Urrutia. **Symposium on Mg Alloys, European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**, Montpellier, France, September 2011.

7. *"Effect of cure cycle on void distribution and mechanical properties of polymer-matrix composites"*, S. Hernández, M. Rodríguez, F. Sket, J. Molina-Aldareguía, C. González, J. LLorca, **Professor K. K. Chawla Honorary Symposium on Fibers, Foams and Composites: Science & Engineering, MST 2011**, Columbus, USA, October 2011.

invited and plenary talks

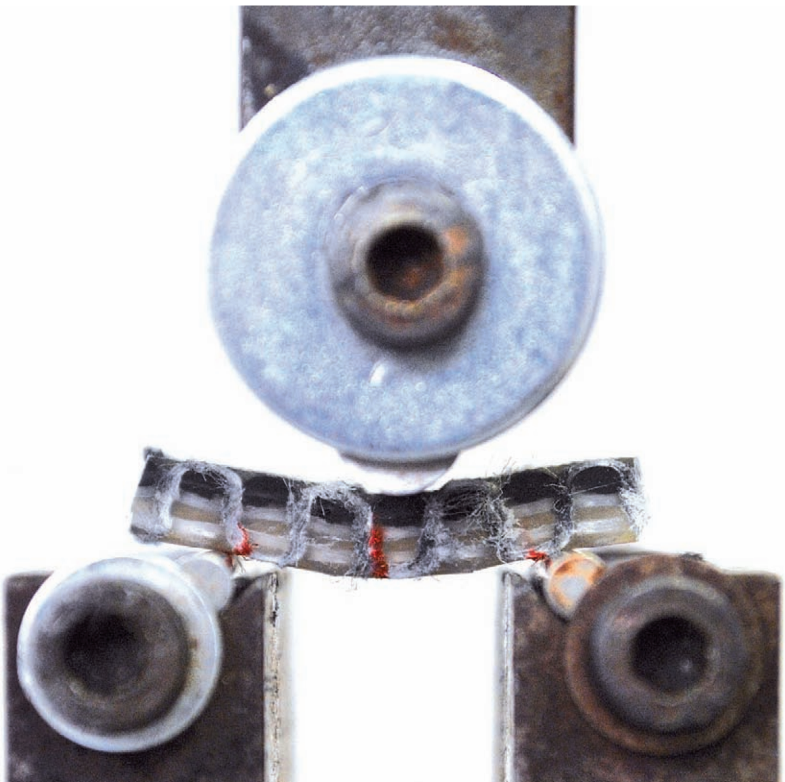
regular contributions

8. *“In-Situ Analysis of deformation and recrystallization mechanisms in Magnesium Alloys”* C. Boehlert, Z. Chen, J. Llorca, I. Gutiérrez-Urrutia, M. T. Pérez-Prado, **Recent Advances in Structural Characterization of Materials: Electron Backscatter Diffraction, MST 2011**, Columbus, USA, October 2011.

9. *“Multiscale modeling of microstructure evolution during cold rolling”*, J. LLorca, J. Segurado, M. T. Pérez-Prado, **Symposium on Multi-scale Modeling of Microstructure Deformation in Material Processing, MST 2011**, Columbus, USA, October 2011.

10. *”Effect of ion irradiation on the micropillar compression of LiF single crystals”*. J. M. Molina-Aldareguia, R. Soler, J. Segurado, J. LLorca, V. M. Orera. **International Conference on Nanomechanical Testing in Materials Research and Development**. Lanzarote, Spain, October 2011.

11. *“Powder Injection Moulding: processing of small parts of complex shape”.* J. M. Torralba, J. Hidalgo, A. Jiménez-Morales. **8th International Conference on Industrial Tools and Material Processing Technologies**. Ljubljana, Slovenia, October 2011.



7.4.2. Regular Contributions

1. *“High performance computational electromechanical model of the heart”*. M. Vázquez, P. Lafortune, R. Arís, G. Houzeaux, A. Jérusalem. **2nd African Conference on Computational Mechanics (AfriCOMP11)**, Cape Town, South Africa, January 2011.

2. *“Void growth in copper during high temperature power law creep”*. K. Dzieciol, A. Borbélya, F. Sket, A. Isaacc, M. Di Michiel, P. Cloetens, Th. Buslaps, A.R. Kaysser-Pyzalla. **ESRF user meeting 2011**, Campinas, Brasil, January 2011.

3. *“Simulation of the through-thickness texture gradient and of the mechanical behavior of pure Zr processed by accumulative roll bonding”*. M. T. Pérez-Prado, J. Segurado, J. LLorca. **Multiscale Modeling of Plasticity (Plasticity 2011)**, Puerto Vallarta, México, January 2011.

4. *“Multiscale modeling of polycrystalline materials: a numerical implementation of the VPSC scheme into an implicit FE code”*. J. Segurado, R. A. Lebensohn, J. LLorca. **Multiscale Modeling of Plasticity (Plasticity 2011)**, Puerto Vallarta, México, January 2011.

5. *“Simulation of damage in composite laminates using X-FEM including experimental validation with X-ray tomography”*. S. Sádaba, R. Muñoz, F. Sket, C. González, J. LLorca. **5th International Conference on Composites Testing and Model Identification (COMPTEST 2011)**, Lausanne, Switzerland, February 2011.

6. *“Characterization of the fiber/matrix interfacial adhesion in fibre reinforced composites by the push-in test”*. M. Rodríguez, J. Molina, C. González, J. LLorca. **5th International Conference on Composites Testing and Model Identification (COMPTEST 2011)**, Lausanne, Switzerland, February 2011.

7. *"Deformation and fracture micro-mechanisms through in situ SEM testing and digital image correlation".* L. P. Canal, C. González, J. Segurado, J. LLorca, **5th International Conference on Composites Testing and Model Identification (COMPTEST 2011)**, Lausanne, Switzerland, February 2011.

8. *"Sequential stages of crack propagation in pre-notched glass fiber/epoxy cross-ply composites studied by XCT".* R. Seltzer, F. Sket, J. Molina-Aldareguía, C. González, J. LLorca, **5th International Conference on Composites Testing and Model Identification (COMPTEST 2011)**. Lausanne, Switzerland, February 2011.

9. *"A discrete dislocation analysis of size effects on void growth in single crystals".* S. Keralavarma, J. Segurado, J. LLorca, A. Benzerga, **2011 TMS Annual Meeting & Exhibition**, San Diego, California, USA, February-March 2011.

10. *"In Situ tomographic characterization of single cavity-growth during high-temperature creep of metallic materials".* A. Isaac, F. Sket, K. Dzieciol, A. Borbely. **2011 TMS Annual Meeting & Exhibition**. San Diego, USA, February-March 2011.

11. *"Exploration of Mg and Ca Based Laves Phases for Hydrogen Storage".* B. Billet, Y. Cui, J. -C. Zhao, L. Bendersky, W. Boettinger. **2011 TMS Annual Meeting & Exhibition**. San Diego, USA, February-March 2011.

12. *"Microtomographic investigation of damage in E911 steel after long term creep".* F. Sket, A. Borbely, K. Maile, R. Scheck. **2011 TMS Annual Meeting & Exhibition**. San Diego, USA, February-March 2011.

13. *"Large scale continuum electromechanical cardiac simulations".* P. Lafortune, R. Arís, M. Vázquez, G. Houzeaux, A. Jérusalem. **2nd International Conference on Mathematical and Computational Biomedical Engineering (CMBE2011)**. Washington DC, USA, March 2011.

14. *"Deformation and damage mechanisms in composite materials by in situ SEM testing".* L. P. Canal, C. González, J. Segurado, J. LLorca, **Deformation and Fracture of Composites 2011**, Sheffield, UK, April 2011.

15. *"Effect of accumulative roll bonding on plastic flow properties of commercially pure Zr".* I. Sabirov, J. M. Molina-Aldareguía, L. Jiang, M. E. Kassner, M. T. Pérez-Prado. **AIP Conference (ESAFORM 2011)**. Belfast, Ireland, April 2011.

16. *"Effect of grain refinement on the mechanical behavior of a 6061 alloy at cryogenic temperatures".* E. Moreno-Valle, M. T. Pérez-Prado, M. Yu. Murashkin, R.Z. Valiev, E.V. Bobruk, I. Sabirov. **AIP Conference (ESAFORM 2011)**. Belfast, Ireland, April 2011.

17. *"Influence of the stress triaxiality and Lode parameter on failure of elasto-plastic porous materials".* P. Ponte Castañeda, K. Danas. **International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC 2011)**. Barcelona, Spain, June 2011.

18. *"An in-situ SEM evaluation of the fracture behavior of a Á-TiAl alloy".* R. Muñoz-Moreno, Y. Cui, J. LLorca, E. M. Ruiz, M. T. Pérez-Prado, C. Boehlert. **12th World Conference on Titanium**. Beijing, China, June 2011.

19. *"Integrated thermo-kinetics database for computational alloy design of the Ti-based alloys".* Y. Cui, H. Chang, J. Li, L. Zhou. **12th World Conference on Titanium**. Beijing, China, June 2011.

20. *"Fibre steering for compression and shear loaded composite panels with cutouts".* V. Gomes, C. S. Lopes, F. Pires, P. P. Camanho, Z. Gürdal. **16th International Conference on Composite Structure (ICCS16)**. Porto, Portugal, June 2011.

21. "*Mechanical testing and simulation of 3D orthogonal interlocked fabric composites*". R. Munoz, R. Seltzer, J. Frontan, C. Gonzalez, J. LLorca. **International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC 2011)**. Barcelona, Spain, June 2011.

22. *"Matrix cracking and crack deflection in unidirectional fiber reinforced composite laminates"*. S. Sádaba, C. González, J. LLorca. **International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC 2011)**. Barcelona, Spain, June 2011.

23. *"Macroscopic instabilities in fiber-reinforced elastomers".* P. Ponte Castañeda, R. Avazmohammadi. **5th International Symposium on Defect and Material Mechanics**. Seville, Spain, June-July 2011.

24. *"Direct observation of repellency of hydrophobic surfaces"*. S. Milenkovic, V. Zaporojtchenko, R. Adelung, F. Faupel, A. W. Hassel. **Engineering of Functional Interfaces (EnFI)**. Linz, Austria, July 2011.

25. *"Matrix cracking and crack deflection in unidirectional fiber reinforced composite laminates".* S. Sádaba, R. Muñoz, F. Sket, C. González, J. LLorca. **MATCOMP 2011**. Girona, Spain, July 2011.

26. *"Variable stiffness composite panels: compression and buckling response"*. O. Falcó, N. Gascons, J. Costa, C. S. Lopes. **MATCOMP 2011**. Girona, Spain, July 2011.

27. *"Damage and defects assessment in composite materials using X-ray computed tomography".* F. Sket, J. Molina-Aldareguia, R. Seltzer, S. Hernández, A. Enfedaque, C. González, J. LLorca. **MATCOMP 2011**. Girona, Spain, July 2011.

28. *"Damage inspection in 3D orthogonal woven composites and plain weave fabrics subjected to both static and impact loads.* Testing and simulation*"*. R. Muñoz, R. Seltzer, F. Sket, C. González, J. LLorca. **MATCOMP 2011**. Girona, Spain, July 2011.

29. *"Damage inspection in 3D orthogonal woven composites and plain weave fabrics subjected to both static and impact loads. Testing and simulation"*. R. Muñoz, R. Seltzer, F. Sket, C. González, J. LLorca. **MATCOMP 2011**. Girona, Spain, July 2011.

30. *"Structure and Properties of Composites of Carbon Nanotube Fibres".* J. J. Vilatela, R. Khare, A. H. Windle. Composite Satellite Meeting of the **12th International Conference on the Science and Applications of Nanotubes**. Cambridge, UK, July 2011.

31. *"Evolution of texture and microstructure of AZ31B Mg alloy sheet at high strain rates".* I. Ulacia, N. V. Dudamell, S. B. Yi, M. T. Pérez-Prado, F. Gálvez, D. Letzig, I. Hurtado. **International Conference on Processing & Manufacturing of Advanced Materials (THERMEC 2011)**. Quebec City, Canada, August 2011.

32. *"Mechanical properties of hybrid stiff coatings deposited onto a polymeric compliant/soft substrate by nanoindentation"*. L. A. Fasce, R. Seltzer, P. M. Frontini. **XIX International Materials Research Congress: Micro and Nanomech**. Cancun, Mexico, August 2011.

33. *"Atomistic modeling of the anisotropic recrystallization of amorphous silicon"***.** I. Martin-Bragado. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

34. "*Constitutive modeling of a neuron under blast loading*". A. Jérusalem, M. Dao. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

35. *"Electrical-mechanical coupling of axons under pressure loading".* J. A. García, S. McHugh, J. M. Peña, A. Jérusalem. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

36. *"Size effects in micropillar compression of LiF single crystals fabricated without exposure to ion irradiation".* J. M. Molina-Aldareguia, R. Soler, J. Segurado, V. Orera, J. LLorca. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

37. *"Characterization of Al-Zn-Mg-Cu/(SiC or TiB_2) composite powders obtained by mechanical milling".* M. A. Jabbari Taleghani, E. M. Ruiz Navas, M. Salehi, J. M. Torralba. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

38. "Simulation of size effects in the growth of cylindrical voids by means of dislocation dynamics and molecular dynamics". J. Segurado, H. J. Chang, O. Rodriguez, B. Martinez, J. LLorca. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

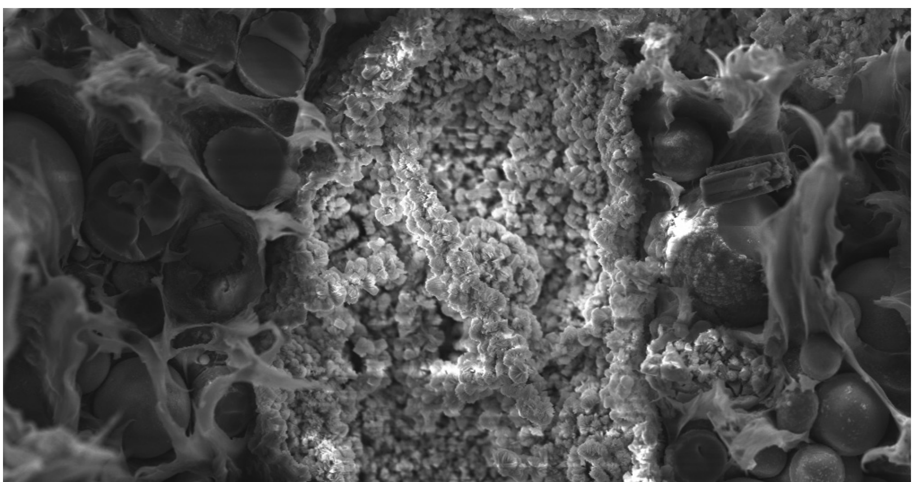
39. *"Multiscale modeling of cold rolling in FCC and HCP metallic alloys".* J. Segurado, J. LLorca, M. T. Pérez-Prado. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

40. *"Lean alloys: from the design to the manufacturing process".* R. Oro, M. Campos, J. M. Torralba. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

41. *"Processing and properties of NiAl-based eutectic composites".* S. Milenkovic, R. Caram, A. Schneider, G. Frommeyer. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. Montpellier, France, September 2011.

42. *"Continuum modeling of Mg alloy AZ31 under uniaxial deformation".* A. Fernández, M.T. Pérez-Prado, Y. Wei, A. Jérusalem. **International Conference on Computational Plasticity: Fundamentals and Applications (COMPLAS 2011)**. Barcelona, Spain, September 2011.

43. *"Influence of hygrothermal aging on the mechanical properties of Nylon 12 composites processed by selective laser sintering".* R. Seltzer, J. Segurado, F. Martin de la Escalera. **5th International Conference on Advanced Research in Virtual and Rapid Prototyping (VRAP 2011)**. Lisbon, Portugal, September 2011.



44. *"Experimental assessment of processing defects on the mechanical properties of a composite material by X-ray tomography"*. S. Hernandez, F. Sket, C. Gonzalez, J. Molina, J. LLorca. **ECCOMAS 3rd Thematic Conference on Mechanical Response of Composites (COMPOSITES 2011)**. Hannover, Germany, September 2011.

45. "Hot workability of an Fe-Al-Nb alloy". S. Milenkovic, I. Sabirov. **Discussion Meeting on the Development of Innovative Iron Aluminium Alloys (FEAl 2011)**. Lanzarote, Spain, October 2011.

46. *"Dynamics of elastic particles in viscous flows"*. P. Ponte Castañeda, T. Gao, H. H. Hu. **48th Annual Technical Conference of the Society of Engineering Science**. Evanston, USA, October 2011.

47. *"Feedstock Development for Powder Injection Moulding of Zirconium Silicate"*. E. Bernardo, J. Hidalgo, A. Jiménez-Morales, J. M. Torralba. **EUROPM 2011**. Barcelona, Spain, October 2011.

48. *"Liquid phase sintering: spreading, wetting and infiltration behavior in a successful reference system, Fe-C-Cu"*. R. Oro, E. Bernardo, M. Campos, J. M. Torralba. **EUROPM 2011**. Barcelona, Spain, October 2011.

49. *"Surface Analysis at Different Sintering Stages of Steel Compacts with Mn and Si"*. R. Oro, M. Campos, E. Hryha, L. Nyborg, J. M. Torralba. **EUROPM 2011**. Barcelona, Spain, October 2011.

50. *"Al-Zn-Mg-Cu/(SiC or TiB_2)p composites developed by powder extrusion: microstructure and mechanical properties"*. M. A. Jabbari Taleghani, E. M. Ruiz Navas, M. Salehi, J. M. Torralba. **EUROPM 2011**. Barcelona, Spain, October 2011.

51. *"Development of new ODS ferritic steels based on Fe-20Cr-5Al prealloyed powders by mechanical alloying"*. N. García- Rodríguez, L. Fuentes-Pacheco, M. Campos, J. M. Torralba. **EUROPM 2011**. Barcelona, Spain, October 2011.

52. *"Homogenization-based constitutive models for electro-active polymers"*. P. Ponte Casteñeda, M. Siboni. **48th Annual Technical Conference of the Society of Engineering Science**. Evanston, USA, October 2011.

53. *"Macroscopic behavior, microstructure evolution and instabilities in nematic elastomers"*. P. Ponte Castañeda, R. Avazmohammadi. **48th Annual Technical Conference of the Society of Engineering Science**. Evanston, USA, October 2011.

54. *"Simulation of failure mechanism of lightweight composite material under impact loading"*. D. D. Tjahjanto, D. Hanumanthappa, A. Jérusalem. **Fifth International Conference on Advanced Computational Methods in Engineering (ACOMEN 2011)**. Liège, Belgium, November 2011.

55. "Magneto-rheological elastomers: Dilute estimates". P. Ponte Castañeda, M. Hakimi-Siboni. **ASME 2011 International Mechanical Engineering Congress and Exposition**. Denver, USA, November 2011.

56. *"Macroscopic instabilities and soft behavior in fiber-reinforced elastomers at finite strain"*. P. Ponte Casteñeda, R. Avazmohammadi. **ASME 2011 International Mechanical Engineering Congress and Exposition**. Denver, USA, November 2011.

57. *"Influence of grain boundary character distribution on mechanical behavior in a nanocrystal multiscale computational model"*. V. Péron-Lührs, A. Jérusalem, F. Sansoz, L. Stainier, L. Noels. **5th International Conference on Advanced Computational Methods in Engineering (ACOMEN 2011)**. Liège, Belgium, November 2011.

7.5. Invited Seminars and Lectures

1. *"Computational materials engineering: an application of multiscale materials modeling"*. J. LLorca. Ira A. Fulton School of Engineering, **Arizona State University**. Tempe, Arizona, USA, January 2011.

2. *"Microstructural development in Powder Metallurgy low alloyed steels"*. J. M. Torralba. Paris-Tech, Centre des Matériaux Pierre-Marie Fourt, **Ecole des mines de Paris**. Paris, France, April 2011.

3. *"Continuum simulation of chemico/electrico-mechanical coupling in individual neurons"*. A. Jérusalem, J. M. Peña. Invited Seminar in **Biotalentum**, Budapest, Hungary, April 2011.

4. *"Virtual testing of structural composites for high performance applications"*. J. LLorca. Institute for Materials Testing, Materials Science and Strength of Materials, **University of Stuttgart**. Stuttgart, Germany, May 2011.

5. *"Thermodynamics modeling, DICTRA-type diffusion modeling for alloy design"*. Y. Cui. **Carlos III University of Madrid**. Madrid, Spain, May 2011.

6. *"New developments in Powder Metallurgy"*. J. M. Torralba. **Fraunhofer-Institut fuer Werkstoffmechanik (IWM)**. Freiburg, Germany, May 2011.

7. *"Integrated computational alloy design for novel rare metal materials"*. Y. Cui. **Southeast University**. Nanjing, China, June 2011.

8. *"Computational alloy design for rare metals and steels"*. Y. Cui. Institute for Structural Materials (ISM), **Central Iron & Steel Research Institute (CISRI)**. Beijing, China, June 2011.

9. *"Multiscale modeling of composites"*. J. LLorca. Department of Materials Science and Engineering, **Carnegie Mellon University**. Pittsburg, Pennsylvania, USA, July 2011.

10. *"Multiscale simulation of structural composites"*. J. LLorca. Department of Materials Science and Engineering, **University of Michigan**. Ann Arbor, Michigan, USA, October 2011.

11. *"Multiscale modeling of composites: a roadmap towards virtual testing"*. J. LLorca. Department of Chemical Engineering and Materials Science, **Michigan State University**. East Lansing, Michigan, USA, October 2011.

12. *"Multiscale modeling of composites: a roadmap towards virtual testing"*. J. LLorca. Materials Research Institute, **Pennsylvania State University**. State College, Pennsylvania, USA, October 2011.

13. *"Multiscale simulation in metallic materials: 2 applications"*. J. Segurado. **Max-Planck-Institut für Eisenforschung Gmbh**. Düsseldorf, Germany, November 2011.

14. *"Multifunctional Nanocomposites based on carbon nanotubes"*. J. J. Vilatela. Department of Physics, **Penn State University**. State College, USA, October 2011.

15. *"Prospects of CNT and graphene composites"*, J. J. Vilatela. Department of Physics, **Universidad Iberoamericana**. Mexico City, Mexico, December 2011.

16. *"Nanocomposites and photocatalytic hybrids based on carbon nanotubes"*, J. J. Vilatela. Department of Chemistry, **Universidad de las Américas Puebla**. Puebla, Mexico, December 2011.

7.6. Organization of Conferences, Workshops and Courses

1. **Plasticity 2012**. J. LLorca, J. Segurado. R. Lebensohn, I. Beyerlein (Symposium organizers on Multiscale Modeling of Plasticity). Puerto Vallarta, México, January 2011.

2. **16th International Conference on Composite Structure (ICCS16)**. C. S. Lopes. (Session Organizer, Composites in Aerospace Applications). Porto, Portugal, June 2011.

3. **Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC 2011)**. J. LLorca, C. González. (Symposium organizers, Multiscale Modelling of Composites). Barcelona, Spain, July 2011.

4. **International Conference on Processing & Manufacturing of Advanced Materials (THERMEC 2011)**. M. T. Pérez-Prado. (Symposium organizer on Severe Plastic Deformation). Quebec City, Canada, August 2011.

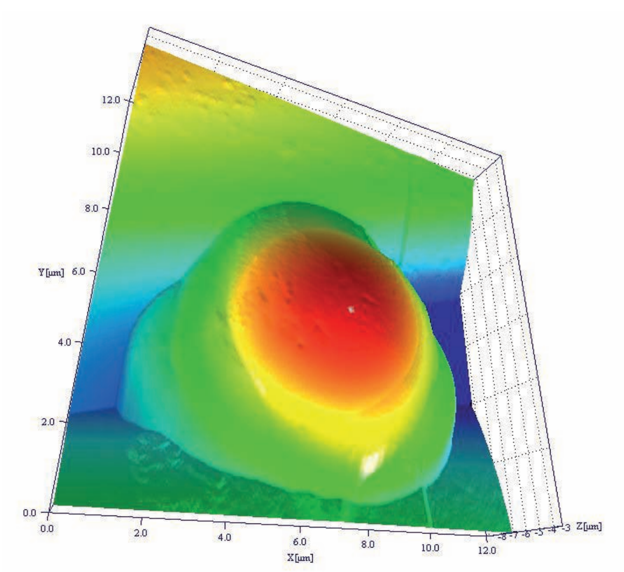
5. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011)**. J. M. Molina-Aldareguia. (Topic Organizer, D3 Materials Modeling on all Length Scales). Montpellier. France, September 2011.

6. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011).** J. Segurado**.** (Symposium Organizer, D32 Modelling of Materials Properties at the Nano and Microscales). Montpellier, France, September 2011.

7. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011).** A. Dasari. (Symposium Organizer, B31 Composites containing Nano-particles and Nano-fibres). Montpellier, France, September 2011.

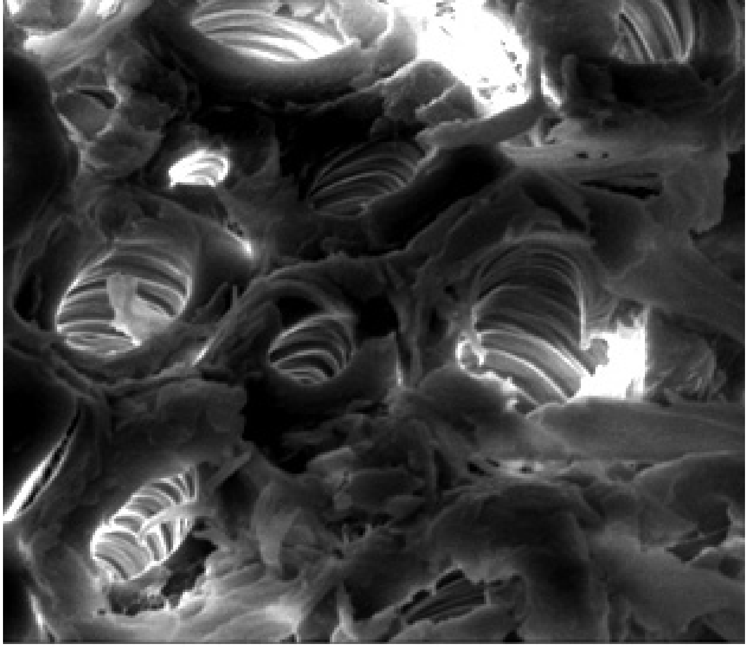
8. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2011).** J. M. Torralba. (Symposium organizer, C31 Powder Synthesis and Processing). Montpellier, France, September 2011.

9. **Graphene in Materials Science.** Regional Meeting. J. J. Vilatela (Chairman). Madrid, Spain, November 2011.



conferences
workshops
courses

7.7. Seminars



1. *"Modelling and simulation for composite materials & process development: points blocking adoption by the aerospace industry".* **S. Van der Veen** (from Airbus Materials & Processes, EDSW, France). January 2011.

2. *"Carbon nanotube fibres and their composites".* **J. J. Vilatela** (from Department of Materials Science and Metallurgy, University of Cambridge, UK). January 2011.

3. *"Damage evolution of texture and microstructure during processing of pure Magnesium and the Magnesium alloy AM30".* **S. Biswas** (from Indian Institute of Science, Bangalore. India). January 2011.

4. *"Damage and failure of non-conventional composite laminates".* **C. S. Lopes**. (from INEGI – Institute of Mechanical Engineering and Industrial Management, University of Porto, Portugal). February 2011.

5. *"The bottom-up chemical approaches in processing of functional nanomaterials".* **O. B. Milosevic**. (from Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Serbia). February 2011.

6. *"Modeling damage accumulation and evolution in fusion materials".* **M. J. Caturla** (from Department of Applied Physics, Universitat d'Alacant, Spain). March 2011.

7. "*Miniaturization: Size effects in plasticity unravelled*". **M. G. D. Geers** (from Department of Mechanics of Materials, Eindhoven University of Technology, The Netherlands). April 2011.

8. *"Structure tensors in nonlinear elasticity: applications to cardiovascular biomechanics and initially-stressed solids".* **R. W. Ogden** (from University of Aberdeen, UK). May 2011.

9. *"Regenerated Bombyx Mori silk: Tuning the structure".* **S. Herrero** (from Department of Materials Science, Polytechnic University of Madrid, Spain). May 2011.

10. *"The pad surface micro-topography and process temperature considerations in planarization".* **A. Philipossian** (from Department of Chemical and Environmental Engineering, University of Arizona, USA). June 2011.

seminars

11. "*Nano-engineered composites".* **R. Guzman de Villoria** (from Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, USA). June 2011.

12. *"Entropic elasticity of fluctuating filaments and networks".* **P. Purohit** (from University of Pennsylvania, USA). July 2011.

13. *"Multi-scale modeling of the mechanical behaviour of polycrystalline ice".* **P. Suquet**. (from Laboratoire de Mécanique et d'Acoustique, CNRS, France). July 2011.

14. *"Design and modification of multifunctional nanomaterial and its polymer nanocomposites".* **D.-Y. Wang** (from Leibniz Institute of Polymer Research, Dresden, Germany). July 2011.

15. *"Using ab-initio based multiscale models and atomic scale experiments for the understanding and design of advanced metallic alloys".* **D. Raabe** (from Max Planck Institute for Iron Research, Dusseldorf, Germany). September 2011.

16. *"Ductile failure at intermediate, high or low stress triaxiality".* **V. Tvergaard** (from Technical University of Denmark, Denmark). October 2011.

17. "*Ge self-diffusion in compressively strained Ge Under a compressive biaxial strain of 0.71%".* **M. Uematsu** (from Keio Univerity, Japan). November 2011.

18. *"Improving Mechanical and Physical Properties of Polymer Nanocomposites".* **Y. W. Mai** (from Centre for Advanced Materials Technology, University of Sydney, Australia). November 2011.

7.8. Fellowships

Amarout Programme, UE-PEOPLE-Marie Curie Cofund, FP7

Call 2011: **Dr. C. S. Lopes, Dr. Y. Cui, Dr. D. Tjahjanto, Dr. M. Monclús**

Call 2010: **Dr. F. Sket, Dr. M. Agoras, Dr. J. Rajakesari, Dr. S. R. Bonta**

Call 2009: **Dr. R. Seltzer, Dr. I. Sabirov, Dr. A. Dasari, Dr. A. Jerusalem**

Ramon y Cajal Programme, Spanish Ministry of Science and Innovation

Call 2011: **Dr. R. Guzman de Villoria, Dr. I. Sabirov**

Call 2010: **Dr. A. Dasari, Dr. S. Milenkovic**

Juan de la Cierva Programme, Spanish Ministry of Science and Innovation

Call 2011: **Dr. J. J. Vilatela, Dr. C. S. Lopes, Dr. S. R. Bonta**

Call 2010: **Dr. R. Seltzer**

Call 2009: **Dr. A. Jerusalem**

China Scholarship Council

Call 2011: **G. Xu, H. Yue**

Cajal Blue Brain Project, Spanish Ministry of Science and Innovation

J. García

Research Stay Grant in Helmholtz Zentrum Geesthacht, Deutsche Akademische Austauschdienst (DAAD)

N. Dudamell

Research Assistant Programme, Madrid Regional Government

M. Rodríguez

7.9. Awards

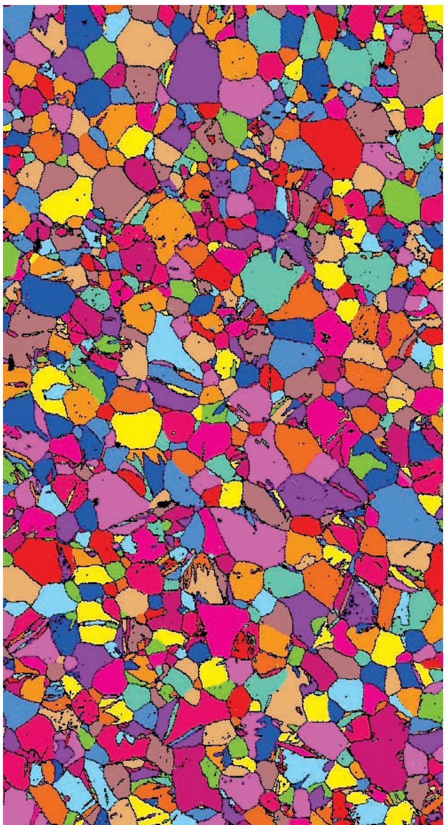
Second prize, best PhD student poster, Aerodays 2011, Madrid, Spain

R. Muñoz

First prize, best PhD student poster granted by the Biointerphases editorial, EUROMAT 2011, Montpellier, France

J. García

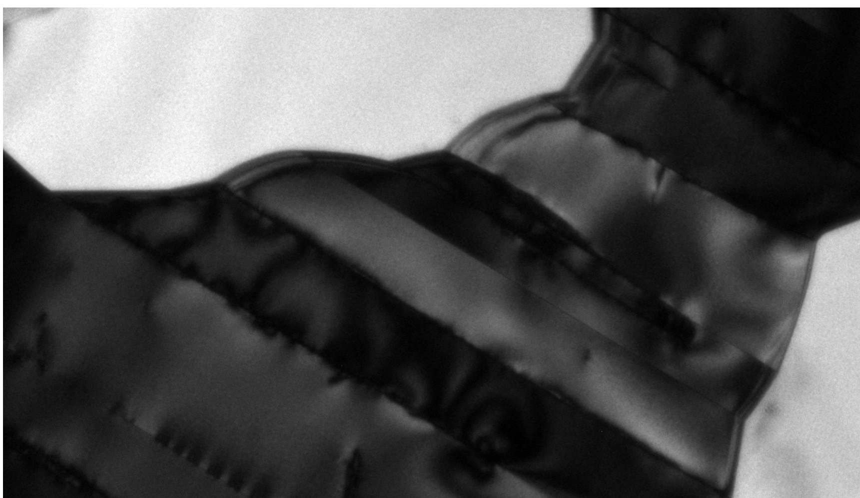
awards



7.10. 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 *Madrid Network.*
- Member of the Network of Research Laboratories of *Comunidad de Madrid* (REDLAB)
- Co-organizers of the *Interuniversity Research Seminars Programme* (P. Laugier, V. Tvergaard and B. van Rietbergen)
- Participation in the "*XI Semana de la Ciencia*", promoted by *Madri+d*
- Participation in the "*Noche de los investigadores*", promoted by *Madri+d*

institutional activities



theses

7.11. Theses

7.11.1. Master/Bachelor Theses

"Morphing materials for aeronautic applications"
Student: Pablo Sorando
Complutense University of Madrid
Advisor: Dr. R. Seltzer
Date: January 2011

"Atomic mobility of the U-Pu-Zr and Ti-Al-Cr ternary alloys"
Student: Weibang Li
Northwestern Polytechnical University, China
Advisors: Dr. Y. Cui and R. Hu
Date: March 2011

"Functional laminates"
Student: Pedro M. Martín
Polytechnic University of Madrid
Advisor: Dr. A. Dasari
Date: March 2011

"Improving the biocompatibility of Zirconium by nanostructuring"
Student: Armind Schmid
University of Bremen, Germany
Advisors: Dr. M. T. Pérez-Prado and A. Dasari
Date: May 2011

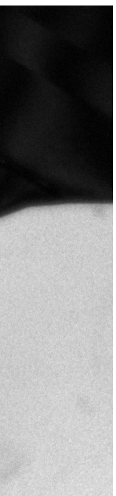
"Delamination damage simulation of composite materials"
Student: J. Javier Lorenzo Cora
Polytechnic University of Madrid and EADS
Advisor: R. Muñoz
Date: December 2011

7.12. Internships / Visiting Students

"Effect of temperature conditions on the strength of recycled prepreg carbon fibers"
Student: Samantha Vitous
Michigan State University, USA
Advisor: Dr. C. González
Date: December 2011

"Tomographic Investigation of ±45° Carbon Fiber Laminates Under Tensile Loading"
Student: Crystal Alton
Michigan State University, USA
Advisors: Dr. F. Sket and Prof. J. Llorca
Date: December 2011

"Study of the compaction effects in VARTM by means of digital image correlations"
Student: Maxime Castillon
INSA Lyon University
Advisors: J. Vila and Dr. C. González
Date: December 2011



internship
visiting students

7.13. Courses

"Introduction to PM"
Course: EPMA 2011 Summer School
Organizer: Fraunhofer Institute IFAM, Dresden, Germany
Professor: Prof. J. M. Torralba

"Simulation techniques"
Course: Master in Composite Materials
Organizer: Polytechnic University of Madrid and EADS
Professors: Dr. A. Jérusalem, Dr. C. González, Dr. J. Segurado, R. Muñoz and S. Sádaba

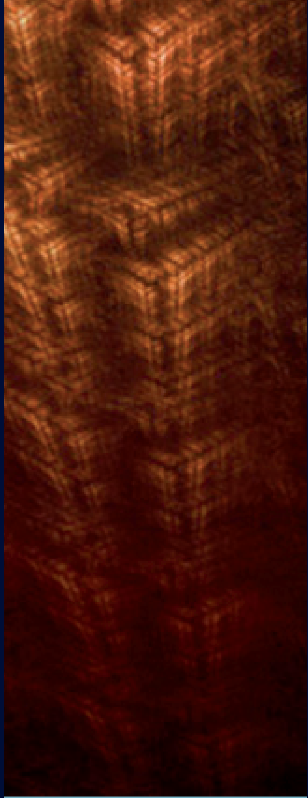
"Non Conventional Composites"
Course: Master in Composite Materials
Organizer: Polytechnic University of Madrid and EADS
Professors: Dr, A. Dasari, Dr. I. Sabirov and Prof. J. Llorca

"Computational mechanics of materials, a continuum perspective"
Course: Master/Doctoral program in advanced computing for science and engineering
Organizer: Polytechnic University of Madrid
Professor: Dr. A. Jérusalem

"Structural Composite Materials"
Course: Master/ Doctoral Program in Engineering of Structures, Foundations and Materials
Organizer: Polytechnic University of Madrid
Professors: Prof. J. LLorca and Dr. C. González

"Mechanics of Composite Materials"
Course: Master/ Doctoral Program in Engineering of Structures, Foundations and Materials
Organizer: Polytechnic University of Madrid
Professors: Dr. J. Segurado and Dr. C. González

courses



8 scientific highlights

Cutting-edge tools for multiscale simulations of failure: Fracture analysis of composite materials

Thanks to the theoretical advances in understanding the complex mechanical behavior of materials and to the progress in numerical methods and computer technology, it is now possible to carry out high fidelity simulations of the mechanical behavior of materials and structures, thus reducing the need for real material testing. In the area of the simulation and analysis of fracture, one of the current challenges is to develop accurate models based on a detailed knowledge of the failure mechanisms at various length-scales. Simplistic models, which ignore the multiscale nature of fracture, might lead to unexpected in-service failures or rely on very conservative assumptions, resulting in oversized, overweighed, cost-inefficient products. IMDEA Materials Institute is aiming at overcoming such limitations by developing multiscale simulation tools based on state-of-the art numerical models for material failure analysis.

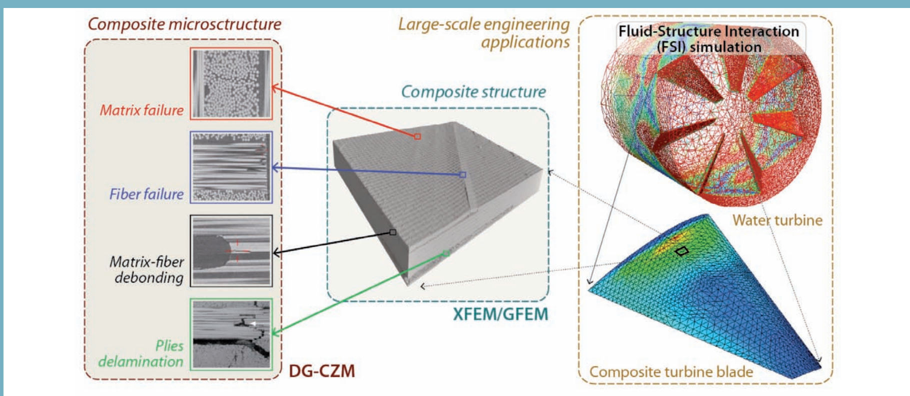


Figure 1. Cutting-edge simulation tools for failure of composite materials in structural applications.

As illustrated in Figure 1, failure of composite materials at microscopic scale is related to three different mechanisms: (i) propagation of crack/fracture in the matrix and/or fibers, (ii) debonding at the matrix/fiber interface, and (iii) delamination between composite plies. Since the topology of fracture is relatively well-determined, material failures at microscopic scale can be modeled with a combination of Discontinuous Galerkin (DG)

scale simulations of failure:

[1] Gmsh is a fully open-source 3D finite element grid generator with a built-in CAD engine and post-processor. Gmsh is developed by Dr. C. Geuzaine and Dr. J-F. Remacle.

method, coupled with an extrinsic Cohesive Zone Model (CZM). As opposed to the classical Galerkin formulation, DG method imposes a weak condition on displacement continuity, eventually replaced by a cohesive law at the onset of fracture. The DG–CZM is implemented on Gmsh[1] in collaboration with Prof. L. Noels and Dr. L. Wu (*University of Liege, Belgium*). Figure 2 shows the predictions of DG–CZM of fracture in a composite ply subjected to transverse loading. In both representative volume element (RVE) samples, failure is dominated by the fracture of the epoxy matrix.

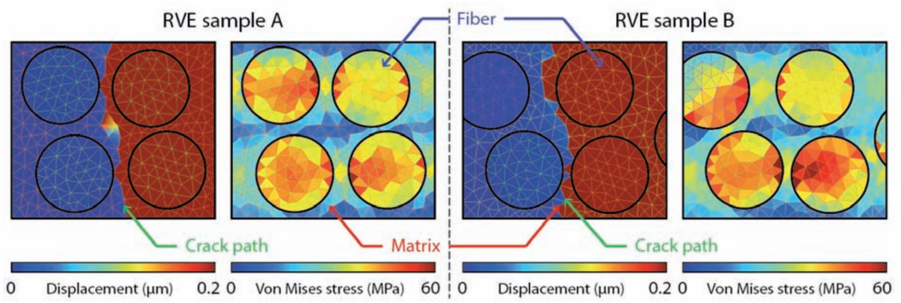


Figure 2. Simulations of fracture in fiber-reinforced composite microstructures using DG-CZM.

[2] Alya is a massively parallel computational framework for solving coupled multi-physic problems, developed and maintained by Dr. M. Vazquez and Dr. G. Houzeaux (Barcelona Supercomputing Center BSC-CNS).

At macroscopic/engineering scale, an eXtended/Generalized Finite Element Method (XFEM/GFEM) is applied to simulate the failure of composite structures. In order to take into account mesoscale discontinuities or cracks, the XFEM/GFEM is enriched by means of Heaviside functions. The XFEM/GFEM is implemented on Alya[2] computational framework, whose high scalability enables a massively parallel XFEM/GFEM implementation suitable for simulating failure of composite materials in full-scale structural components. As an example, Figure 3 shows examples of XFEM/GFEM simulation of mode I and mode II crack opening in a composite plate with their corresponding stress distribution.

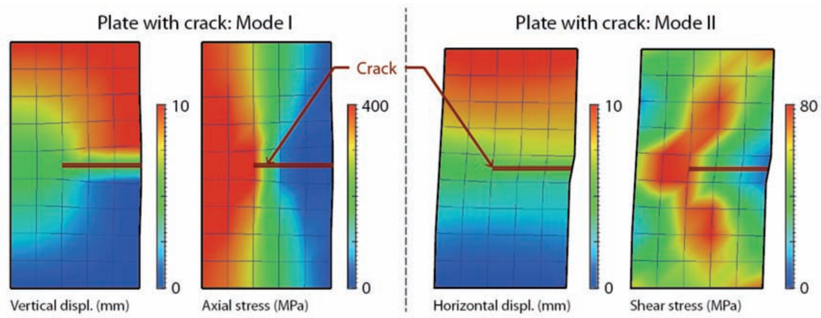


Figure 3. Simulated displacement and stress fields of macroscopic crack evolution in composite coupons using XFEM/GFEM.

atomistic modeli

recrystallization for microelectronic applications

Atomistic modeling of the silicon recrystallization for microelectronic applications

The current push of society for more powerful and advanced microelectronic gadgets is nowadays truer than ever. This appetite, together with the impressive opportunities of semiconductor devices in new areas, such as biomedical applications, keeps the interest in the research on Si-based materials after several decades of continuous success.

In particular, amorphization of the Si lattice by heavy-ion implantation, and subsequent recrystallization by solid phase epitaxial regrowth (SPER) is widely used in the most advanced devices. Recent examples are the fabrication of field effect devices (FETs) or the current interest in SPER activation of dopants for low temperature fabrication of vertical integrated devices.

(a) *(b)*

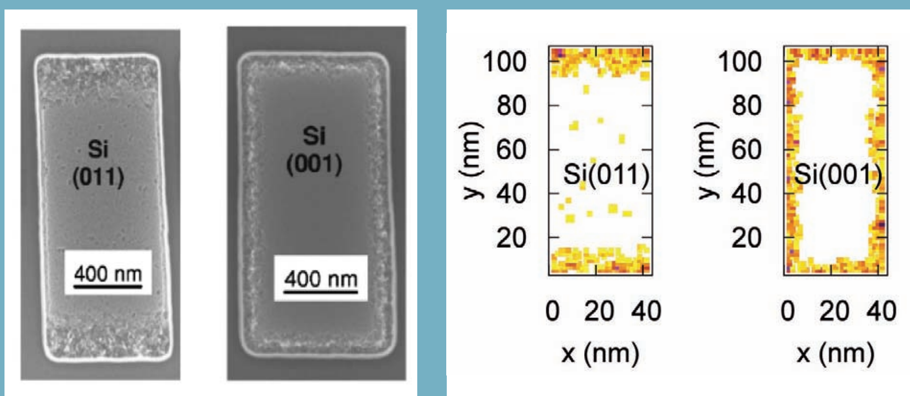


Figure 1.(a) Experimental results of defect formation after SPER (from [1]). (b) Numerical simulations obtained with the atomistic Lattice Kinetic Monte Carlo model [2]. Two cases are shown, including two defective edges in a (011) substrate and four defective edges in a (001) Si substrate, both aligned with <110> axes.

In order to improve the understanding of SPER, a research team of IMDEA Materials Institute has developed an atomistic Lattice Kinetic Monte Carlo model that replicates the process of defect formation during SPER. The new module has been implemented in

ng of the silicon

the modular Monte Carlo simulator MMonCa developed at IMDEA Materials Institute. The main model assumption is that {111} microscopic facets in the material produce defective Si by allowing the local formation of twin defects [2], which influence the overall SPER evolution, shape and interface roughness [3].

(a) *(b)*

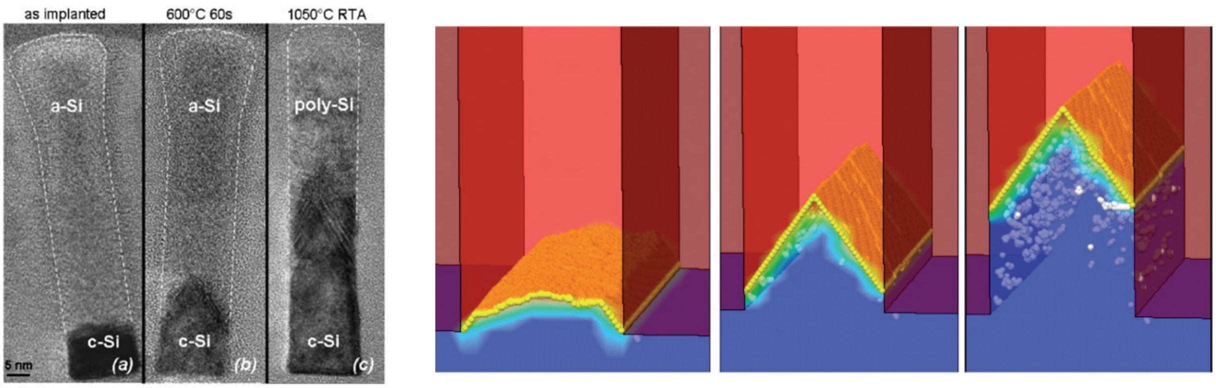


Figure 2.(a) Experimental results of a sub-20 nm wide silicon fin after a) amorphization, b) subsequent 600ºC, 60s annealing and c) 1050ºC annealing (TEM images taken from Ref. [4]) (b) cross-section of the simulated defect morphology during SPER at 600ºC of a small 20x60 nm² thin Si fin surrounded by SiO_2. [2], [5]

References

[1] K. L. Saenger et al. A study of trench-edge defect formation in (001) and (011) silicon recrystallized by solid phase epitaxy. *J. Appl. Phys, 101,* 024908, 2007

[2] I. Martin-Bragado. {111} local configurations: The main source of silicon defects during solid phase epitaxial regrowth modeled by Kinetic Monte Carlo. *Applied Physics Letters, 98,* 233109, 2011

[3] I. Martin-Bragado. Importance of twin defect formation created by solid-phase epitaxial growth: an atomistic study. *Scripta Materialia, 66,* 186-189, 2012

[4] R. Duffy et al. Solid phase epitaxy versus random nucleation and growth in sub-20 nm wide fin field-effect transistors. *Applied Physics Letters, 90,* 241912, 2007

[5] Image produced with *Sentaurus* Process, 2012.

seeking mult

Seeking multifunctionality using nanomaterials

using nanomaterials

Start at the bottom

As a consequence of their size and atomic structure, nanomaterials have a range of unique properties often not found in the bulk. They include boron nitride (BN) nanotubes with stiffness of ~ 1TPa, carbon nanotubes (CNTs) with thermal conductivity of ~ 3000 W/mK and an electrical conductivity close to that of copper, graphene layers with specific surface area of 2630 m^2/g. Researchers at IMDEA Materials work actively in the synthesis of nanomaterials with novel morphologies and molecular structure, and with a wide range of properties (mechanical, electrical, thermal, photocatalytic,etc) that can be exploited for multifunctionality. Figure 1 shows an example of microcoils consisting of CNTs assembled into double helices, grown by chemical vapour deposition on conventional metals (steel, copper, etc) [1]. The helical morphology can be induced by controlling the substrate-catalyst particle interaction.

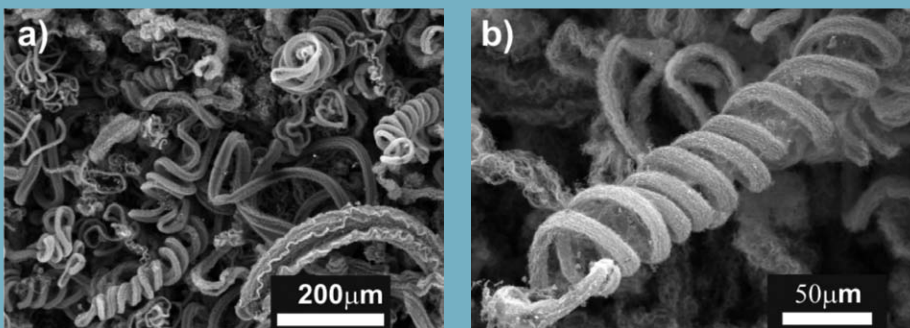


Figure 1. Scanning electron micrographs of carbon nanotube double helices [1]

These nanomaterials have potential applications as reinforcement in composites with very large strain-to-failure, resonating elements, electromagnetic wave absorbers, microsensors, micro/nano-electromechanical systems (MEMS or NEMS) and, in general, where large energy absorption by mechanical deformation is sought. Current efforts are focused on better controlling their growth and on incorporating them in composites.

Integration in composites

In order to exploit the outstanding properties of nanomaterials on a macroscopic scale, it is necessary to integrate them into larger structures, either through their incorporation into a matrix, or by assembling them as a macroscopic object. At IMDEA Materials, we follow three different integration routes depending on the application (Figure 2). In the first type, the nanocarbon is used as a filler added to a polymer matrix, while the second consists of hierarchical composites with macroscopic fibres and nanocarbon in a polymer matrix; the third type are nanocarbon-based macroscopic fibres which can then be processed to form standard fibre-reinforced polymer composites. See our recent review article on "Nanocarbon Hybrids and Composites in Sustainability" for more details [2].

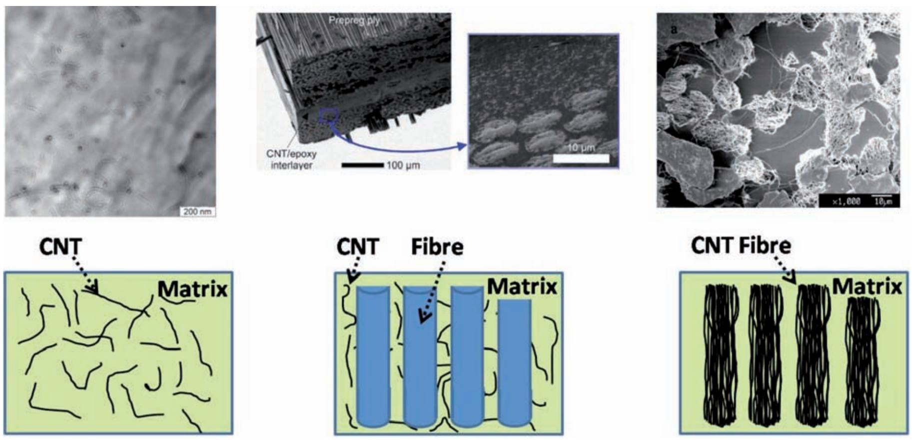


Figure 2. Schematic of different methods of exploiting the properties of nanomaterials (CNTs) on a macroscopic scale: As fillers (a), in FRP to form a hierarchical composite (b), or as part of CNT-based fibres (c). Electron micrographs from [3],[4],[5]

Example: Improvement of carbon fibre composites through addition of carbon nanotubes

Through the addition of CNTs to the resin, it is possible to improve the mechanical properties of the composite and provide additional functionality in the form of electrical and thermal conductivity. The CNTs are first dispersed in the epoxy using high shear forces applied by calendering; subsequently the CF fabric is impregnated with modified resin and then cured (Figure 3).

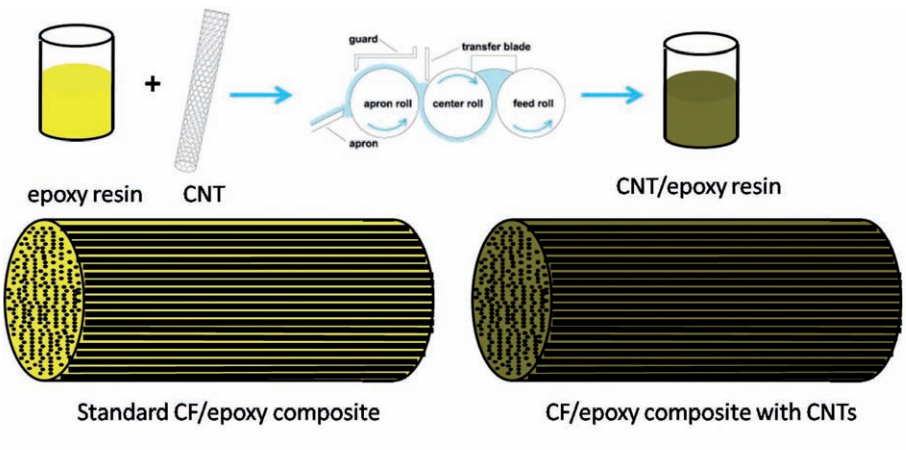
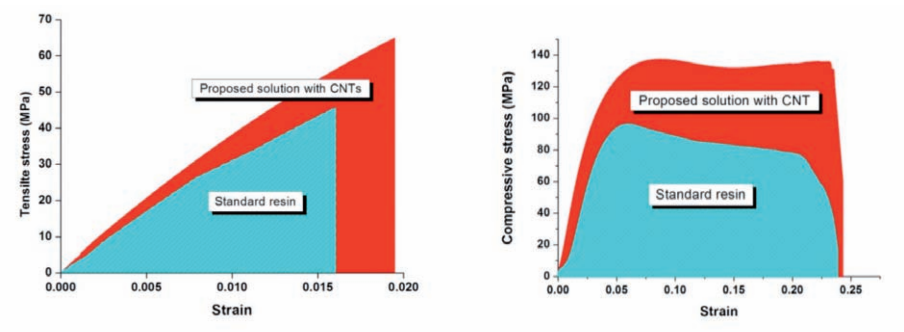


Figure 3. Schematic showing the integration of CNTs in hierarchical CF composites

The comparison of properties of CF composites manufactured with the standard resin and the new resin containing CNTs is shown below. Better mechanical and electrical properties are obtained by means of the dispersion of CNTs and further improvements are expected through the development CNT/CF/epoxy hierarchical composites.



Property	Standard resin		CNT-modified resin	
	Tension	Compression	Tension	Compression
Young´s modulus (GPa)	3.2	2.4	3.7	2.8
Maximum stress (MPa)	42	94	57	134
Strain at maximum stress (%)	1.5	7.2	1.9	9.2
Electrical conductivity (S/m)	-	0.02		

References

[1] F. Cervantes, J. J. Vilatela, L. G. Reyes et al. Carbon nanotube bundles self-assembled in double helix microstructures. *Carbon*, *50*, 1227-1234, 2012

[2] J. J. Vilatela, D. Eder. Nanocarbon composites and hybrids in sustainability: a review. *Chem. Sus. Chem.*, *5,* 456-478, 2012

[3] E. Logakis, P. Pissis, D. Pospiech, A. Korwitz, B. Krause, U. Reuter, P. Pötschke. Low electrical percolation threshold in poly(ethylene terephthalate)/multi-walled carbon nanotube nanocomposites. *European Polymer Journal*, *46,* 928-936, 2012

[4] E. J. Garcia, B. L. Wardle, A. J. Hart. Joining prepreg composite interfaces with aligned carbon nanotubes. *Composites: Part A*, *39,* 1065-1070, 2008

[5] R. J. Mora, J. J. Vilatela, A. H. Windle. Properties of composites of carbon nanotube fibres. *Comp. Sci. Tech.*, *69,* 1558-1563, 2009

High temperature nanomechanical testing: ...or the art of compressing pancakes...

...or the art of compressing pancakes...

Researchers at IMDEA Materials Institute are pioneering the development of novel high temperature nanomechanical testing techniques in order to study the mechanical properties of materials at the micro and nanoscale. The objective is two-fold. On the one hand, these techniques are necessary to study size effects in the mechanical properties of materials, relevant for applications in which miniaturization is leading to smaller and smaller devices. On the other hand, they open the door to screen the mechanical properties when the amount of material available is so limited that conventional testing is precluded.

Micropillar compression tests, in which a microscopic pillar of the material is compressed on a dedicated nanoindentation platform, is a good example of this strategy (Fig. 1). Micropillar compression at room temperature has been proven an effective method to study size effects in the deformation and fracture mechanisms of very small volumes of metallic materials, of the order of 1 μm^3, but the extension of such tests to high temperature is still an uncharted world. This is due to the difficulty of achieving the required thermo-mechanical stability to measure loads and displacements with nanoNewton and nanometer resolution, respectively.

A current example of application of these tests is found in the case of nanoscale multilayers. These materials, consisting of alternating layers of two materials, are attractive composites due to their unique electrical, magnetic, optical, and mechanical properties. In particular, metal-ceramic systems, like Al/SiC, display an attractive combination of strength, hardness and toughnes. However, little is known about their high temperature mechanical behavior as they are manufactured in the form of very thin (≈ µm) coatings on Si substrates by magnetron sputtering and there are not standard methods to test their high temperature mechanical properties.

Researchers at IMDEA Materials Institute have overcome this limitation by using Focused Ion Beam machining to fabricate micropillars of 500 nanometers in diameter, that were deformed in compression using a high temperature nanoindentation system. The images in Fig. 1 show two micropillars compressed at ambient temperature and 100ºC, highlighting the large difference induced by temperature in the behavior of the confined plastic defor-

[1] In collaboration with Prof. Chawla, Arizona State University

mation of the metallic layers[1]. At room temperature, the compressive strength of the multi-layers was very large (≈3 GPa) as a result of the constrained plastic deformation of the nanometer thick metallic layers confined between the stiff ceramic layers. However, the enhanced plastic flow of the nanostructured Al layers at 100ºC (showed by the large extrusions on the edges of the micropillars, Fig. 1b) led to a large reduction in strength. The study reveals the mechanisms at the microscale responsible for the attractive combination of strength and toughness, but also highlights the large sensitivity to the temperature, that results in a 50% reduction in strength at 100ºC (Fig. 2), due to the nanostructure of the Al layers.

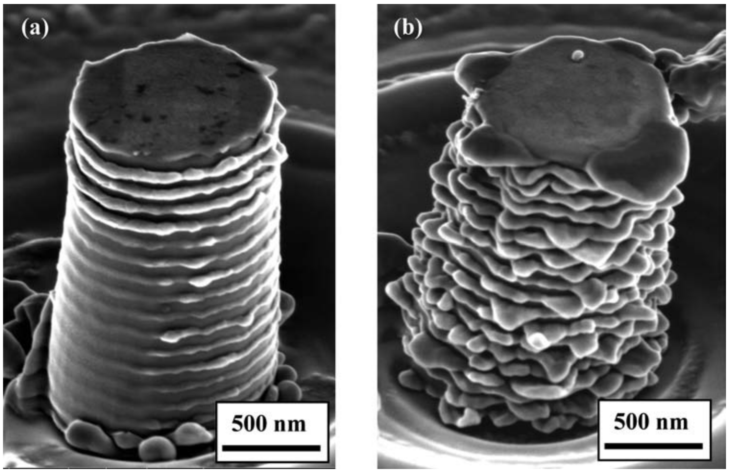


Figure 1. SEM image of compressed micropillars of nanoscale Al/SiC multilayers at: (a) room temperature and (b) 100ºC.

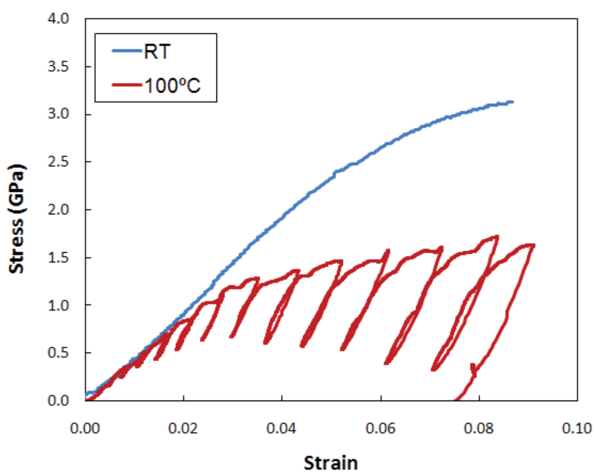


Figure 2. Compressive stress-strain curves of Al/SiC nanoscale multilayers at room temperature and 100ºC.

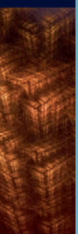
Multiscale modeling of plasticity: application to forming processes

application to forming processes

Engineering alloys are heterogeneous materials formed by aggregation of grains with different orientation of one or more metallic phases. Plastic deformation occurs by dislocation and/or twinning in each microscopic grain and depends on the grain orientation, size and shape, the stresses acting on the grain, and the constraint imposed by the deformation of the neighbor grains. From a macroscopic viewpoint, the plastic flow of engineering alloys is usually modeled by means of phenomenological models (such as J_2 or Drücker-Prager), which parameters can be obtained from simple tension tests. These models cannot establish, however, the relationship between the microstructure and the macroscopic behavior (because of their phenomenological foundation) and its accuracy is doubtful during processes in which the grain size, shape and orientation changes dramatically during deformation, as in the case of many forming processes (rolling, forging, ECAP, etc.).

To overcome these limitations, IMDEA Materials Institute – in collaboration with Los Alamos National Laboratory – has developed a novel multiscale modeling tool to simulate the plastic deformation of polycrystalline materials at the microscopic and macroscopic scales [1]. The simulation tool is based in a continuum crystal plasticity approximation of the grain deformation at the microscopic scale. At the macroscale, each point of the solid corresponds to a polycrystal formed by a few hundred grains and its plastic response is obtained using a homogenization technique (the visco-plastic self-consistent scheme [2]). This information is used within the framework of the finite element model to determine the macroscopic mechanical response. The macroscopic fields provided by the finite element analysis are used as input to compute the deformation of each polycrystal in which the evolution of the microstructure is updated during the simulation (Fig. 1).

The new tool is able to carry out accurate simulations of complex forming processes such as cold rolling, forging or ECAP. For instance, the simulation of cold rolling of a 6061 Al alloy sheet is depicted in Fig. 2. The finite element model is able to incorporate the macroscopic details (cylinders size, rolling speed, friction, etc.), while the microstructure at each point is represented by a polycrystal containing 500 grains whose shape and orientation evolves during the simulation. Thanks to the multiscale approach, both macroscopic fields and microscopic information are solved simultaneously and, for instance, the grain orientation distribution (texture) in each point of the sheet is obtained, Fig 2(c).



ling of plasticity

Macroscale (sample) *Microscale*

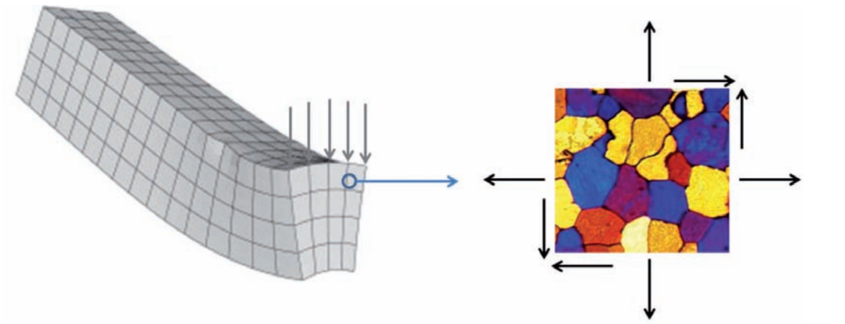
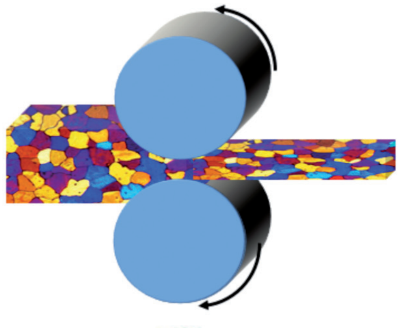


Figure 1: Multiscale modeling framework to simulate the plastic deformation of polycrystalline engineering alloys [1]. (a) Macroscale, where the global geometry and boundary conditions of the solid are defined and (b) Microscale representing the polycrystalline microstructure at each point of the solid.

a)

b)



c)

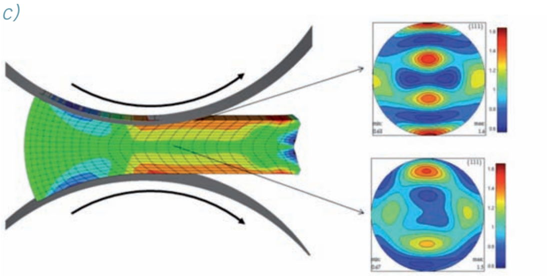


Fig 2: (a) Actual rolling of an Al alloy plate. (b) Schematic of the rolling process (c) Multiscale simulation of cold rolling of an Al alloy with 50% of reduction. The pole figures corresponding to the <111> direction are shown for two points (near the center and near the surface) of the plate.

References

[1] J. Segurado, R. A. Lebensohn, J. Llorca, C. N. Tomé. Multiscale modeling of plasticity based on embedding the viscoplastic self-consistent formulation in implicit finite elements. *Int. J. Plasticity, 28,* 124-140, 2012

[2] R. A. Lebensohn, C. N. Tomé. A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: Application to zirconium alloys. *Acta Metall. Mater, 41,* 2611-2624, 1993

editor
imdea materials institute

graphic design
base 12 diseño y comunicación

D.L.
M-14.944-2012

www.materials.imdea.org

La Suma de Todos
Comunidad de Madrid
www.madrid.org

EUROPEAN UNION
STRUCTURAL FUNDS

madrid institute
for advanced studies

institute
imdea
materials

www.materials.imdea.org

Contact
contact.materials@imdea.org
tel. +34 91 549 34 22
fax +34 91 550 30 47

E.T.S. de Ingenieros de Caminos
C/ Profesor Aranguren, s/n
28040 Madrid, Spain