madrid institute
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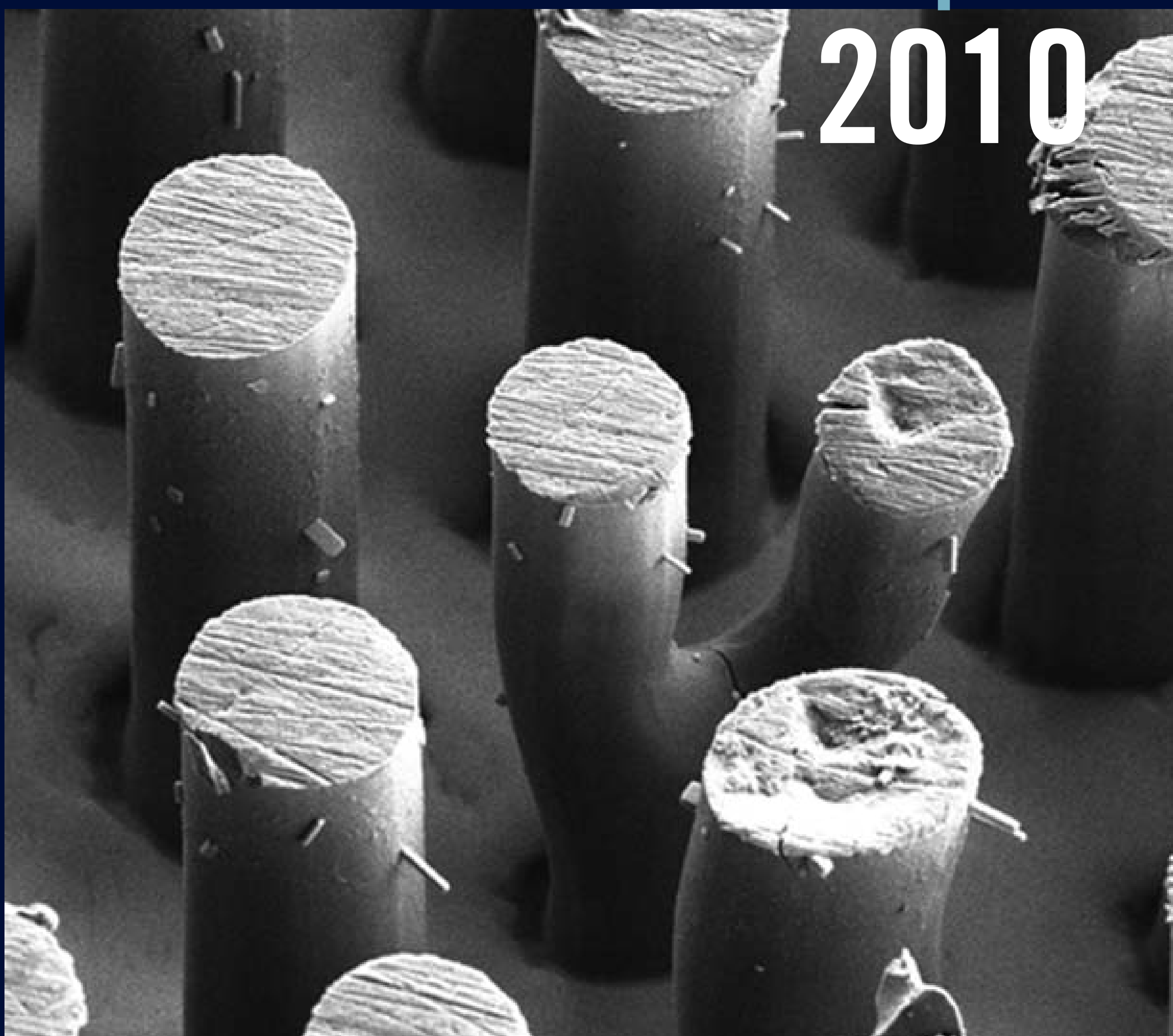
institute
imdea
materials

annual report 2010



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annual report 2010

foreword

foreword

Javier LLorca
Director IMDEA Materials Institute
May 2011

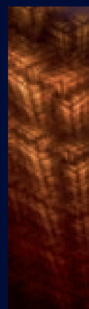
word

If I were to summarize in one word the activities of IMDEA Materials Institute in 2010, the most appropriate one would be ‘expansion’. The Institute has grown in all fronts and has grown swiftly upon the solid foundations laid in previous years. Firstly, new talent has been incorporated to the Institute, which currently counts with 7 senior researchers and 8 researchers who lead 14 different research lines. They are supported by 7 postdoctoral research associates and 17 doctoral students, leading to a total of 39 researchers from 13 different nationalities. At this point, 50% of the scientists working in IMDEA Materials have been born outside of Spain and 60% of the PhD theses were granted by foreign universities, establishing IMDEA Materials as a truly international research institution. New talent has also been added to the Scientific Council with the incorporation of four new members (Prof. J. R. Willis, Cambridge University; Prof. J. E. Allison, University of Michigan; Prof. Y.-W- Mai, University of Sydney; and Prof. W. A. Curtin, Brown University). They will provide advice and guidance to maintain scientific excellence in the core of the activities. Finally, Prof. Suresh and Prof. Pinnavaia resigned as Board and Council Members because of incompatibilities with their new positions as Director of the National Science Foundation of the US and Executive Vice-president of InPore Technologies, respectively. This is the place to thank them for their time and support during these initial years.

Another important growth event was related to the physical space. On April 19th, Mrs. Esperanza Aguirre, President of the Madrid Regional Government, laid the first stone for the construction of the building of IMDEA Materials Institute at the Scientific and Technological Park of the Polytechnic University of Madrid in TecnoGetafe. Construction is running on schedule and will be finished by the end of 2011, providing the facilities and laboratories necessary to maintain the competitiveness of the Institute at international level.

Growth was also indicated by the number of publications in peer-reviewed international journals (32), patents (3) and competitive research projects funded by the Madrid Regional Government, Spanish Ministry of Science and Innovation (7) and the European Union (8). Moreover, direct technology transfer to industry has been carried out through 6 research projects funded by industrial companies. Last but not least, IMDEA Materials Institute potential has increased with the opening of two new research laboratories devoted to nanomechanics and to the physical simulation of processing of metallic alloys.

Finally, the Institute activities were evaluated for the first time by the international Scientific Council. The overall performance of the Institute during the period 2007-2010 was rated excellent because the primary objectives (research of excellence, technology transfer to industry and attraction of talent) were achieved in full. In addition, the Scientific Council issued a number of recommendations, which will guide the scientific activities of the Institute in the following years.



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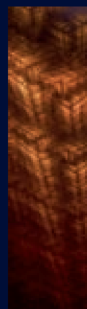
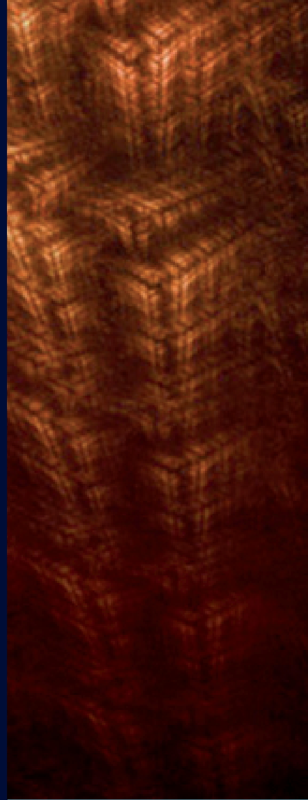




1

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 objectives: 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. Incorporations to the Scientific Council

The Board of Trustees appointed four new scientists to the Scientific Council with a well-established international reputation in three research areas of the institute. They are Prof. John R. Willis (Department of Applied Mathematics, Cambridge University), Prof. Yiu-Wing Mai (School of Aerospace, Mechanical and Mechatronic Engineering, University of Sydney), Prof. William A. Curtin (School of Engineering, Brown University) and Prof. John E. Allison (Department of Materials Science and Engineering, University of Michigan). These appointments enhance the current expertise of the Scientific Council in the areas of Mechanics, Multifunctional Composites and Nanocomposites, Multiscale Materials Modelling and Physical Metallurgy.

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

1.3. Management Structure

Since September 2010, the management structure of the Institute has been reinforced with the incorporation of a Personnel Manager whose main responsibilities include supporting and facilitating new researchers from abroad besides supporting administrative staff in other areas.

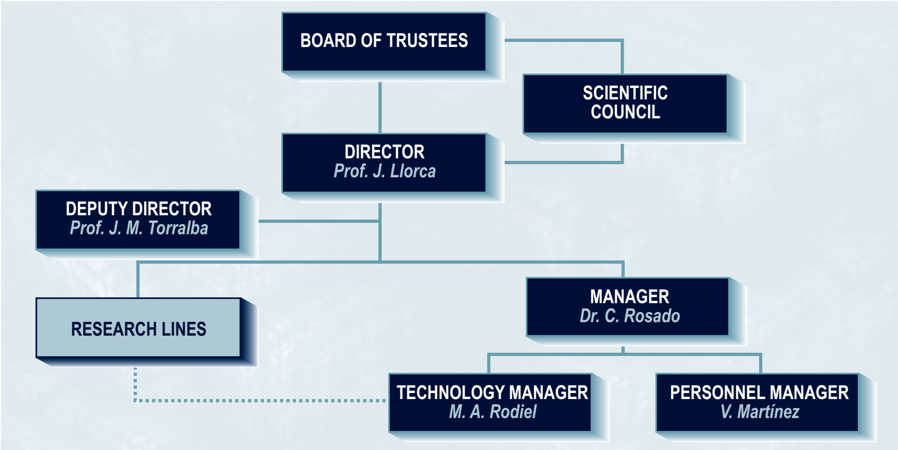


Figure 1. Management Structure

1.4. Beginning of the Institute Construction

On April 19th 2010, Mrs. Esperanza Aguirre, President of the Madrid regional government, laid the first stone of the construction of the building of IMDEA Materials Institute at the Scientific and Technological Park of the Polytechnic University of Madrid in TecnoGetafe. The building has a total floor area of 9.000 m^2 devoted to office space for management and researchers, seven research laboratories (processing of nanocomposites, processing of advanced structural materials, chemical and microstructural characterization, thermo-mechanical characterization, nanomechanics and computational materials science), as well as a conference area to host scientific workshops. The construction is expected to be finished by November 2011.

Figure 2. Mrs. Esperanza Aguirre, president of the Madrid regional government, during her speech at the Ceremony of the placement of the first stone of the building of IMDEA Materials Institute

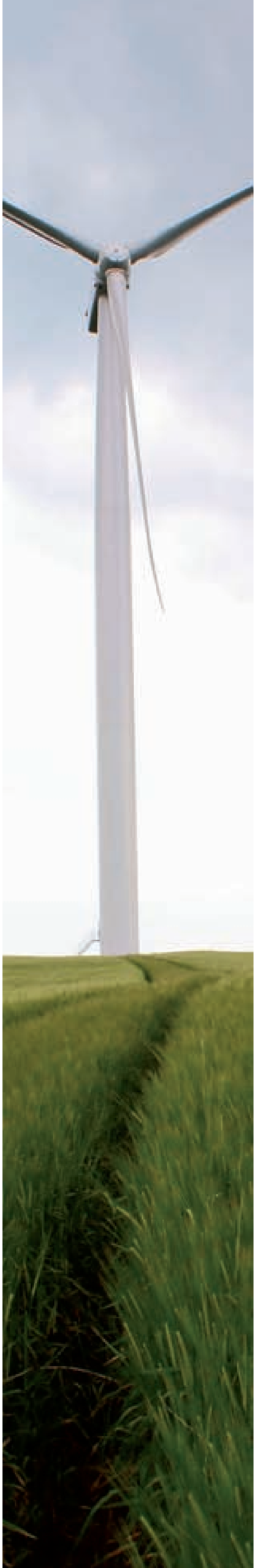
TecnoGetafe, a scientific and technological park created by a joint venture of the Madrid regional government and the municipality of Getafe, is located at sixteen kilometres to the south of Madrid city. With an area close to 1 million of square meters, it is one of the largest in Europe and its activities are focussed in the areas of aerospace/aeronautics, engineering, energy and new technologies. Together with industrial enterprises, 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 (in which IMDEA Materials Institute is located) includes the university research centres on aerospace engineering, industrial engineering, as well as earth, energy and materials engineering and Centesil, a pilot plant devoted to the purification of Si for photovoltaic solar cells.

Figure 3. Construction of IMDEA Materials Institute

Up until the final building is available, IMDEA Materials Institute is developing its activities in two provisional sites. The first one, located at the School of Civil Engineering of the Polytechnic University of Madrid, hosts the offices for the director and staff belonging to the Divisions of Composite Materials and Modelling & Simulation as well as the research line on Nanomechanics and Micromechanics. The second one, located at the Carlos III University of Madrid, hosts the Division of Metallic Materials and the research line on Multifunctional Nanocomposites.

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. England

Prof. Trevor W. Clyne
Professor
Cambridge University. UK

Prof. William A. Curtin
Director of the Center for Advanced Materials Research
Professor
Brown University. USA

Prof. Manuel Elices
Professor
Polytechnic University of Madrid. Spain

Prof. Toribio Fernández Otero
Professor
University of Cartagena. 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 of the Centre for Advanced Materials Technology (CAMT)
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
Deputy Director
FIDAMC. Spain

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

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

Prof. Gary Savage
Mercedes GP. UK

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

Prof. John R. Willis
Professor
Cambridge University. UK

performance evaluation

2

Following the Articles of Association, the institute activities during the first four years (2007-2010) along with the performance of the staff scientists during 2009-2010 were evaluated by the Scientific Council in the meeting held in Madrid on 18th November, 2010.

The basic criteria analysed by the council members to assess the institute performance were the following:

- Personnel: incorporation of scientists, attraction of talent, international reputation (leadership, awards, fellowships, invited/keynote contributions in international conferences, etc.).

- Scientific results: quality and impact, publications in peer-reviewed international journals and patents.

- Research lines: opening and development of research lines, installation of research infrastructures, interdisciplinary and international character of the research environment.

- Research projects: funding, funding bodies, industrial partnership and technology transfer, international collaborations, etc.

The overall performance of the institute during the period 2007-2010 was rated excellent because the primary objectives of the Institute (research of excellence, technology transfer to industry to maintain competitiveness and attraction of talent) were achieved. In addition, the Scientific Council issued a number of recommendations, which were approved by the Board of Trustees. They include:

- The development of closer links with a few key industrial partners, particularly multinational companies.

- Exploratory research of high visibility and/or added value should remain the primary aim of the Institute. The current balance between such "A-class" research activity and funding attraction should be maintained.

- The Institute should take appropriate measures to retain the talent attracted thus far.

- Closer links should be developed with the surrounding academic environment and the institute should position itself as a resource for neighbouring universities and research centres.

Chart 1. Number of reseachers

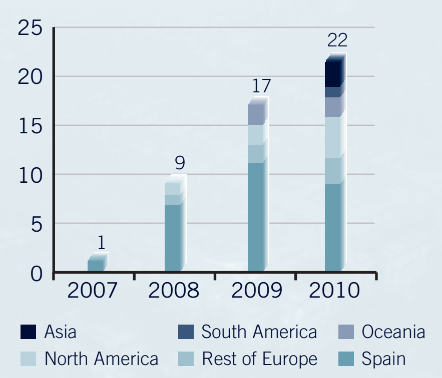


Chart 2. Country of the PhD degree

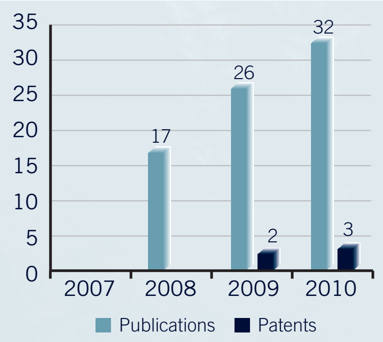


Chart 3. Publications in international peer-reviewed journals and patents

Chart 4. Active research projects by funding source

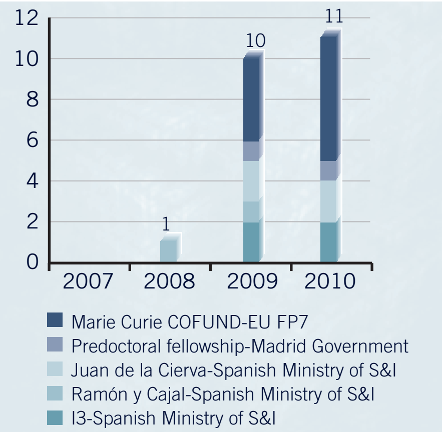
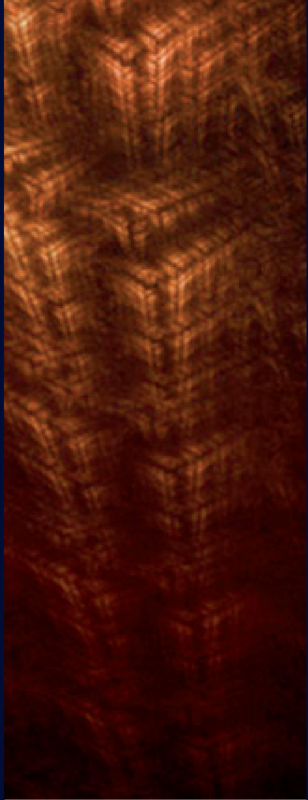


Chart 5. Fellowships and grants



3 research

3.1. Research Lines

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

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

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

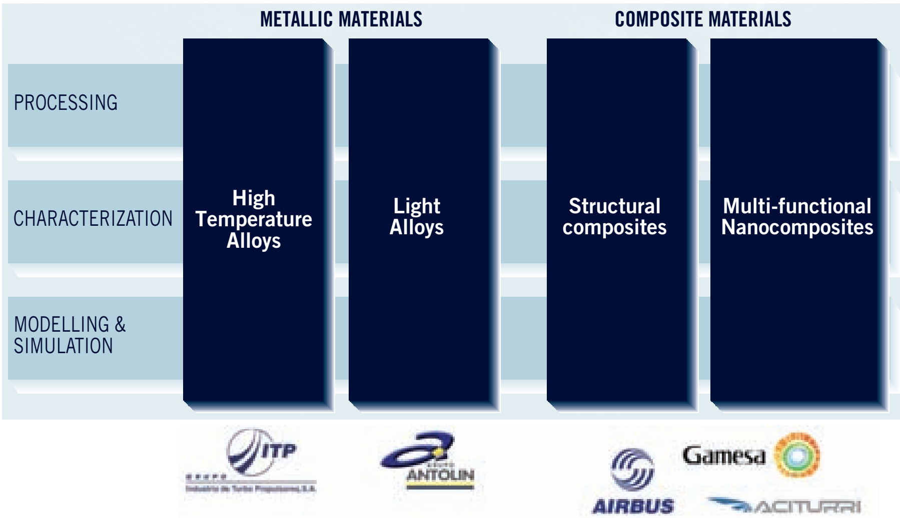


Figure 4. Vertical and horizontal research lines of IMDEA Materials Institute

3.2. Research Activities

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

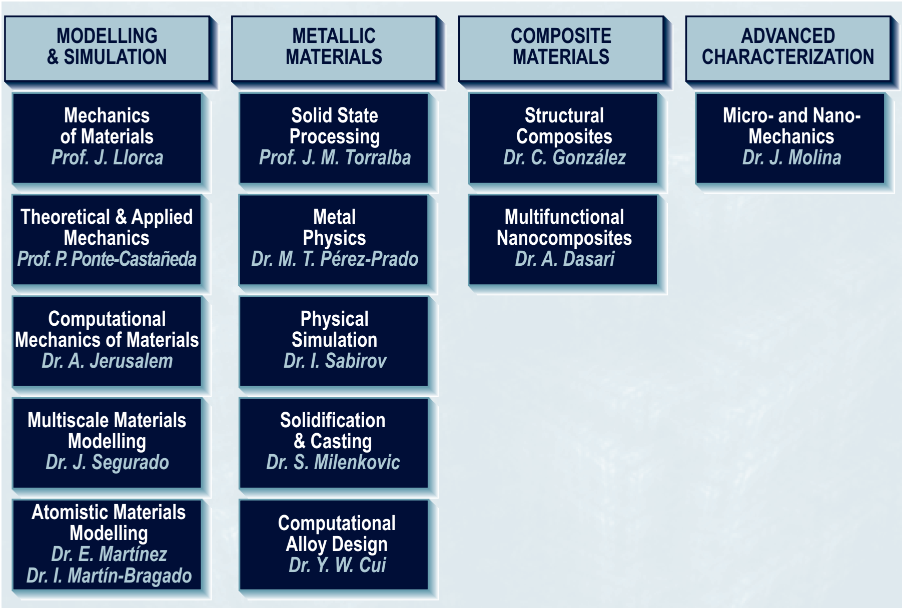


Figure 5. Research groups of IMDEA Materials Institute

3.2.1. Modelling & Simulation

This research division encompasses five research groups: **Mechanics of Materials** (Prof. J. LLorca), **Theoretical and Applied Mechanics** (Prof. P. Ponte-Castañeda), **Computational Mechanics of Materials** (Dr. A. Jérusalem), **Multiscale Materials Modelling** (Dr. J. Segurado) and **Atomistic Materials Modelling** (Dr. I. Martin-Bragado and Dr. E. Martínez). Together, the expertise of the five research groups covers all the relevant simulation strategies to model the mechanical behaviour of materials from atomic scale to the dimensions of actual components, including *ab initio*, molecular mechanics, kinetic Monte Carlo, dislocation dynamics, finite elements and homogenization theory. Main research activities are focussed in the development of advanced tools and simulations strategies to carry out virtual tests of composites and metallic materials, prediction of size effects in the mechanical behaviour at the nm-μm scale and understanding the behaviour and structural evolution of neurons upon mechanical loading.

3.2.2. Metallic Materials

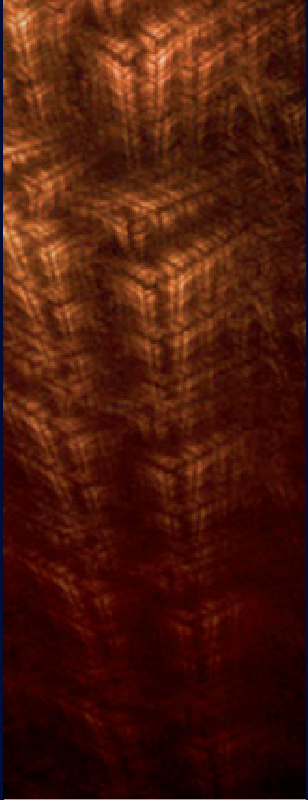
The activities of IMDEA Materials in the area of Metallic Materials are distributed in five research groups devoted to **Solid State Processing** (Prof. J. M. Torralba), **Metal Physics** (Dr. M. T. Pérez-Prado), **Physical Simulation** (Dr. I. Sabirov), **Solidification and Casting** (Dr. S. Milenkovic) and **Computational Alloy Design** (Dr. Y. Cui). Research activities in this line cover a wide range of processing techniques for engineering alloys (including powder metallurgy, directional solidification and casting, welding, severe plastic deformation, etc.), physical simulation of the influence of processing parameters on the microstructure, analysis of the relationship between the microstructure and mechanical properties and virtual design of new alloys with optimized properties by means of computational thermodynamics.

3.2.3. Composites

The activities of IMDEA Materials in the area of composite materials are performed by two research groups on **Structural Composites** and **Multifunctional Nanocomposites** led by Dr. González and Dr. Dasari, respectively. 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, biocide activity, etc.). In addition, 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.

3.2.4. Advanced Characterization

This research line, led by Dr. J. M. Molina-Aldareguía, is focused on **advanced characterization techniques at the nm and μm level**. In addition to standard techniques for microstructural characterization (TEM, SEM, X-ray diffraction, TGA, DSC, spectroscopy, etc.), a leading objective is to develop novel experimental methods to quantify mechanical properties at the nm and μm level. Current activities 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, experimental determination of size effects on the flow strength of ceramic nanopillars and characterization of defects and voids at the microscale by means of X-ray computer-assisted microtomography.



4 people

After the last International Call launched in 2010, IMDEA Materials Institute currently counts with 39 researchers, including 6 Senior Researchers, 1 Visiting Scientist, 8 Researchers, 7 Postdoctoral Researchers, and 17 Predoctoral Researchers from 13 different nationalities. Approximately 50% of the researchers have been born abroad.

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. José Manuel Torralba

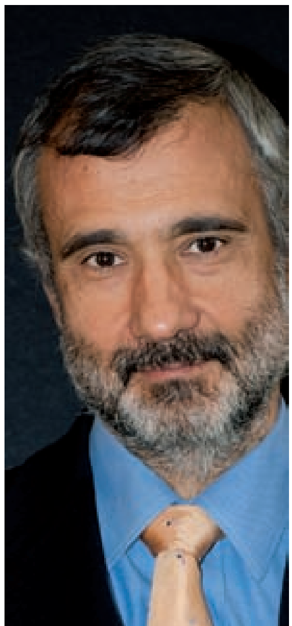
Deputy Director,
Solid State Processing

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 aluminum, 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 Molina
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 another line of interest is the fabrication of novel metallic phases with improved mechanical and functional properties by compression and shear.

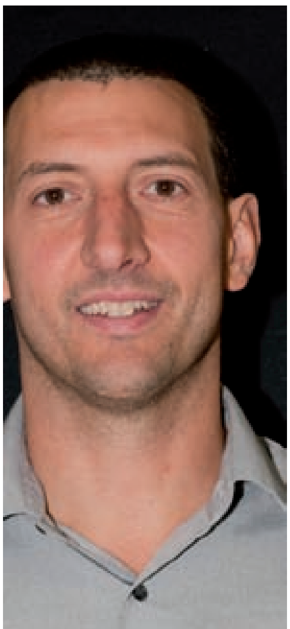
Prof. Pedro Ponte Castañeda
Associated Senior Researcher, Theoretical and Applied Mechanics

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,
High-temperature Alloys

Ph.D. in Materials Science and Engineering from University of Dayton. USA
Associate Professor in the Department of Chemical Engineering and Materials Science, Michigan State University

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. Aravind Dasari

Researcher, Multifunctional Nanocomposites

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

Research Interests

Electrospinning technique, processing-structure-property relationships of polymeric materials and more specifically, thermal stability/flame retardancy, tribology, and deformation/fracture mechanisms of polymer nanocomposites. He continues to work towards obtaining new generation of multi-functional and environmentally-friendly materials.

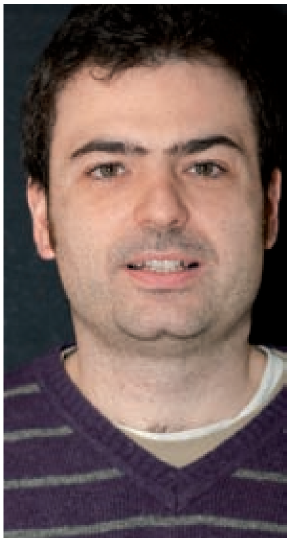
Dr. Antoine Jérusalem

Researcher, Computational Mechanics of Materials

Ph.D. in Computational Mechanics of Materials from Massachusetts Institute of Technology. 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. Enrique Martínez

Researcher, Computational Materials Science

Ph.D. in Nuclear Engineering from Lawrence Livermore National Laboratory, USA

Research Interests

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

Dr. 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.

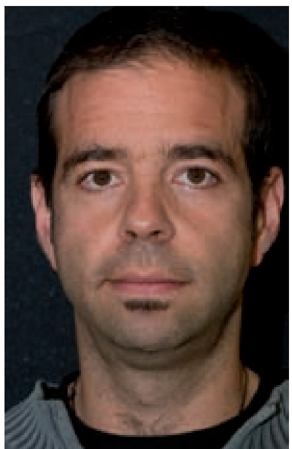
Dr. Javier Segurado

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 micromechanics strategies to simulate the mechanical behaviour until failure of both particle and fibre reinforced composites.



new incorporations to staff researchers

Dr. Yuwen Cui

Researcher, Computational Alloy Design

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

Dr. Cui received his MSc and PhD in Materials Science from Central South University in 1995 and 1999, respectively. Following postdoctoral research from 1999 to 2003 at Tohoku University and Katholieke Universiteit Leuven (Belgium), he joined the National Institute of Advanced Industry Science and Technology at Tohoku Center (Japan) as an AIST Special Researcher in April 2003; then moved to Tohoku University as COE Fellow/Senior CREST Researcher in April 2005. He joined the Ohio State University in May 2008 as a Research Associate, where he worked until he joined IMDEA Materials Institute as a Researcher. He is the author of over 30 research articles in peer-reviewed international journals and has recently co-authored one book chapter in "Computational Methods for Microstructure-Property Relationships". He received the Award of Excellence of the Hunan province (China) for his PhD thesis, the COE Research Fellow Grant from Tohoku University in 2005 and 2006, the Catholic University of Leuven Council Award in 2001 and 2002, and the Marie Curie AMAROUT Incoming Fellowship from the European Union in 2010.

Research Interests

Dr. Cui's current research focuses on computational thermodynamics (i.e. CALPHAD) and kinetics, high throughput diffusion research and diffusion modelling, and microstructural simulation by using the Landau theory and phase field model. His research work has led to the development of commercial thermodynamics databases and the computational alloy design of Pb-free micro-solders, Ni-base superalloys and the new generation of Co-based high temperature alloys and he is also working in the development of lightweight interstitial alloys for hydrogen storage.

Dr. Ignacio Martín-Bragado

Researcher, Atomistic Materials Modelling

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

Dr. Martin-Bragado completed his MSc in Physics at the University of Valladolid in 1998 and got his PhD in Physics from the same university in 2004. His PhD dissertation on "Atomistic Process Simulation for Microelectronics" captured the interest of Synopsys Inc, and he joined the company to develop the atomistic process simulator "Sentaurus Process KMC". After six months working in Munich, Germany, he moved to Mountain View in October 2005 as the R&D leader for Sentaurus Process KMC. The simulator entered the market in 2006 and is considered the most advance tool for simulation of TCAD processing of semiconductor materials. It includes models for impurity and dopant diffusion, activation and deactivation of dopants, extended defect formation, stress and strain dependencies, local Fermi-level corrections, dynamic annealing, amorphization, isothropic and anisothropic solid phase epitaxial regrowth, etc. It is currently used by the leading microelectronic fabrication companies, including IBM, Freescale, Taiwan Semiconductor Manufacturing Company, Panasonic, Global Foundries, Fujitsu, Samsung, Texas Instruments, etc. Dr. Martín-Bragado has participated in 9 research projects (4 as principal investigator) and has co-authored more than 30 papers in peer-reviewed international journals.

Research Interests

Current research interests of Dr. Martin-Bragado include the 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 and development of other atomistic (*ab initio*) and multiscale simulation techniques.

Dr. Srdjan Milenkovic

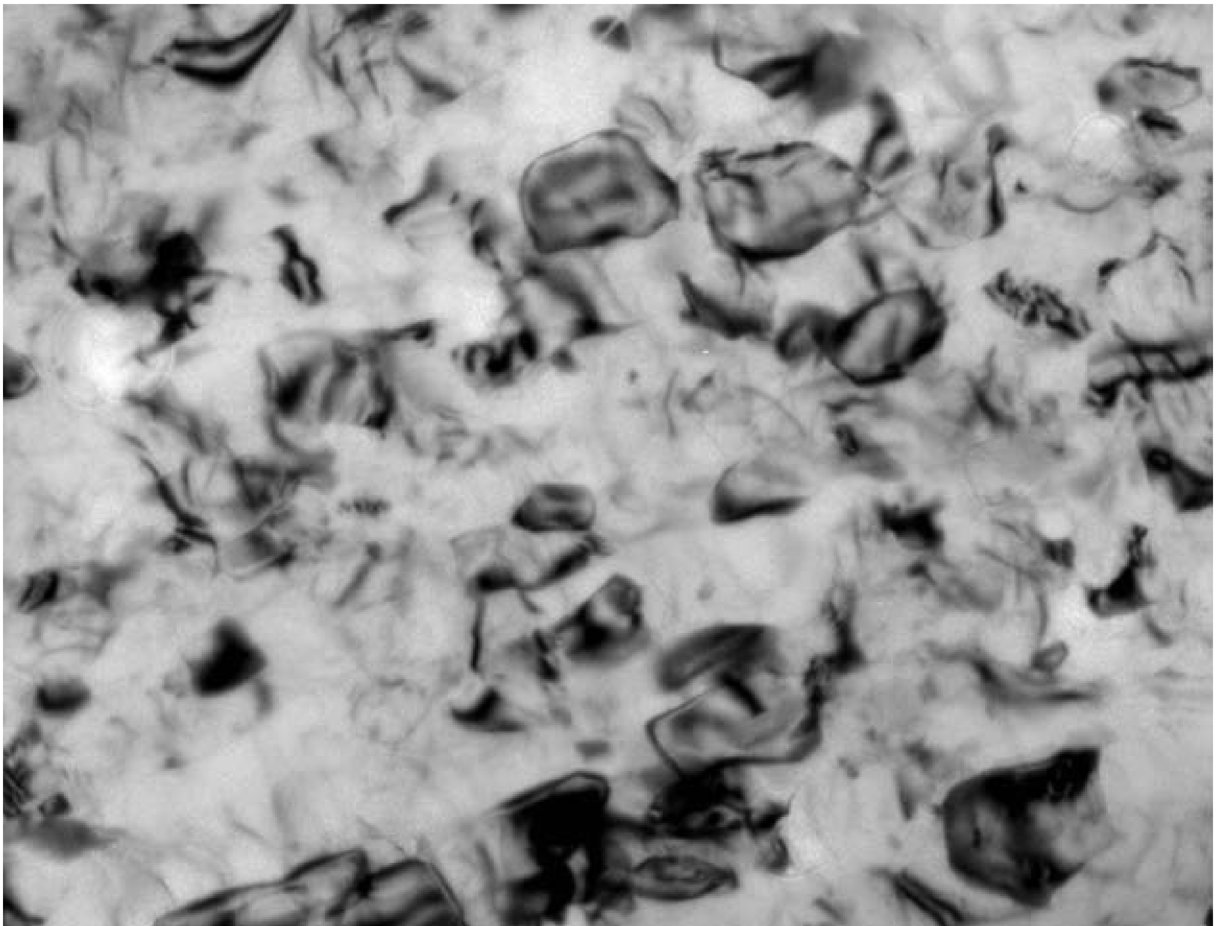
Researcher, Solidification and Casting

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

Dr. Srdjan Milenkovic graduated with a B.Sc. degree in Metallurgy from Belgrade University (Serbia) in 1995. He received his MSc and PhD degrees in Materials Engineering in 1998 and 2002, respectively, from the State University of Campinas (Brazil). Upon completion of his PhD, he obtained a prestigious fellowship of the Max-Planck-Society for Advancement of Science for a Postdoctoral research position at the Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf (Germany) under supervision of Prof. Frommeyer. In 2004, he joined the Department of Interface Chemistry and Surface Engineering at the same Institute, as a Research Associate and later on as a head of nanotechnology laboratory. Before joining IMDEA Materials as Researcher in 2010, he was head of the nanotechnology lab and lecturer at the Institute for Chemical Technology of Inorganic Materials, Johannes Kepler University in Linz (Austria). Dr. Milenkovic has authored or co-authored more than 40 papers in peer-reviewed international journals. Based on his scientific track record, position in the field, and contributions to the science and technology of advanced materials, he was recently included in the 2010 Edition of "Who's Who in the World" and 2010 IBC Edition of "Top 100 Scientists". His research experience has evolved through various research projects, funded both by industry and national and European funding programmes. He has received the Ramon y Cajal grant from the Spanish Ministry of Science and Innovation (2010).

Research Interests

His research interests are twofold. The first one is focused on 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. The second research field of interest is nanotechnology in general, and more specifically synthesis and characterization of metallic nanowires through directional solidification and electrochemical treatment of eutectic alloys.



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. 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. More specifically, his interests include the stabilization of high pressure phases in pure Zr and pure Ti by the application of shear under pressure.

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. She has also expertise in fillers for rubber formulations, organically-modified nanoclays and flame retardant additives.

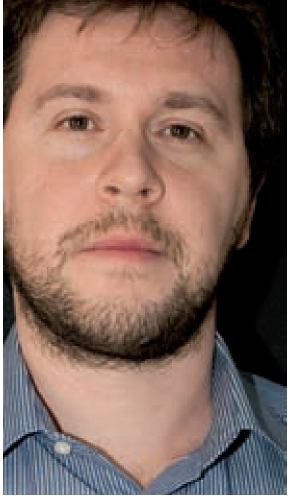
Dr. Jerome Rajakesari

Postdoctoral Research Associate

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

Research Interests

Multiscale modelling of electrical conductivity of carbon nanotubes reinforced polymer-matrix composites from nm to continuum level to predict and design the electrical properties lightning impact resistance of carbon nanotubes reinforced polymer-matrix composites.


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.

Dr. Federico Sket
Postdoctoral Research Associate

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

Research Interests

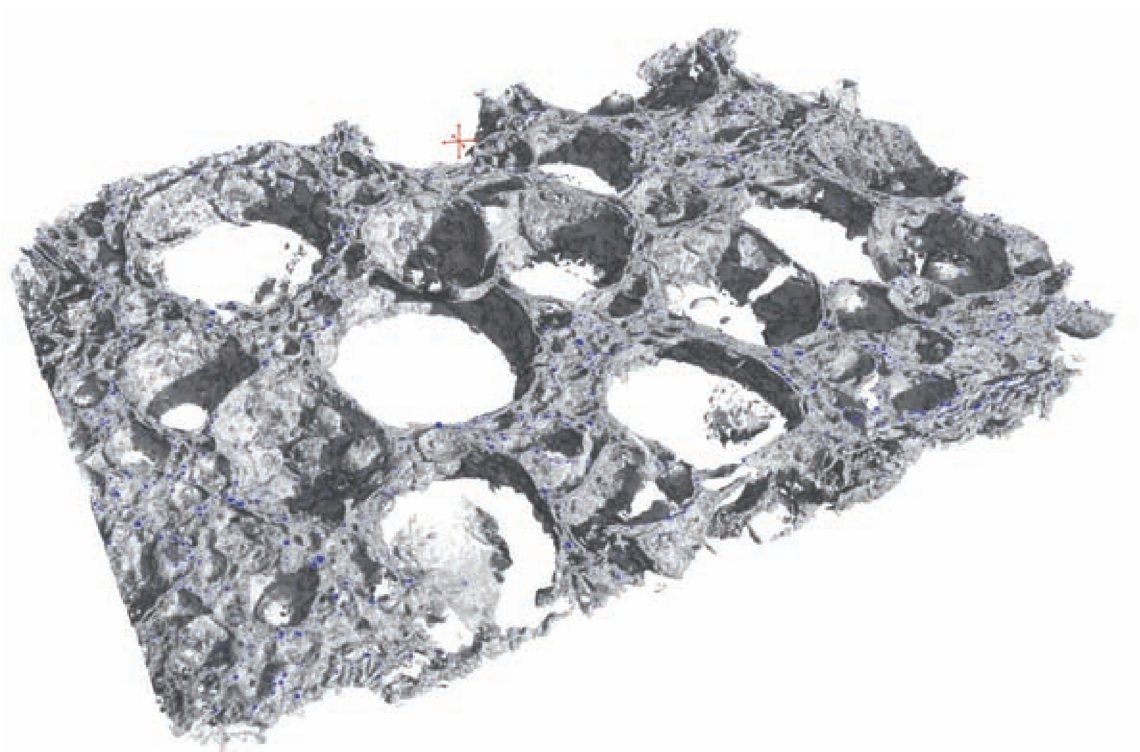
Mechanical characterization and the application of X-ray microtomography to understand and characterize the deformation and damage mechanisms of advance structural materials.

Dr. Katia Tamargo
Postdoctoral Research Associate

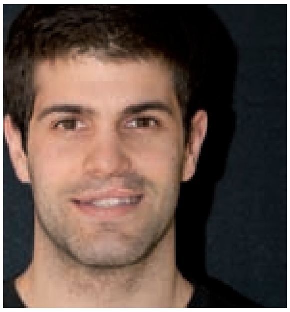
Ph.D. in Chemistry of Materials from University of Oviedo, Spain

Research Interests

Properties of high-performance polymeric fibres (PBO, PPTA), with particular emphasis on the interfacial adhesion with epoxy matrices to improve the mechanical properties of composites. Surface modification of polymer fibres via plasma treatments, characterization of physical, chemical and mechanical properties of the modified fibres, and preparation and mechanical characterization of polymer-matrix composites.



predoctoral research assistants




Sergio Arias

M.Eng.: Carlos III University of Madrid. Spain
Research: Nanomechanics

Nathamar Dudamell

M.Eng.: Central University of Venezuela. Venezuela
Research: Physical metallurgy of Mg alloys

Rainer Eberle

M.Eng.: Zurich University of Applied Sciences. Switzerland
Research: Composites processing

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

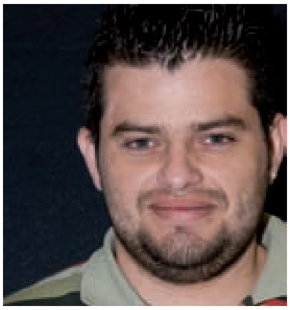
M.Eng.: University of Stuttgart. Germany
Research: Numerical simulation of composites impact

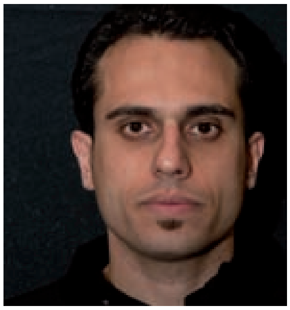
Silvia Hernández

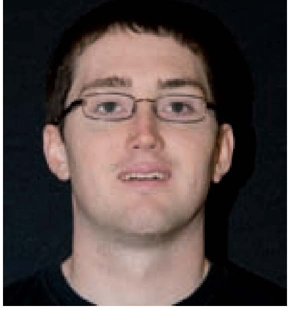
M.Sc.: Complutense University of Madrid. Spain
Research: Processing of composite materials

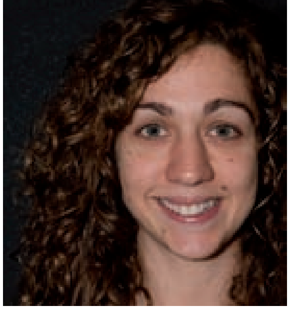
Mohammad Ali Jabbari

M.Eng.: Isfahan University of Technology. Iran
Research: Solid state processing







Saeid Lotfian

M.Eng.: Isfahan University of Technology. Iran
Research: Nanomechanics

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

Rocio 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 materials

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

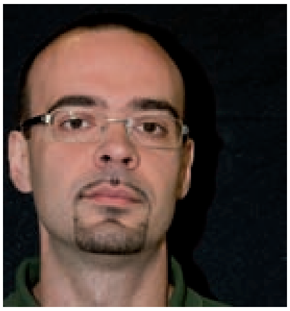
Rafael Soler

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

Joaquim Vilà

M.Eng.: University of Girona. Spain
Research: Structural composites

laboratory technicians



José Luis Jiménez

V.T.: Specialist Technician. Spain

Vanesa Martínez

M.Eng.: University of Valencia. Spain

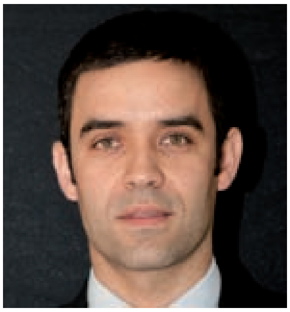
Juan Carlos Rubalcaba

B.Eng.: Alcalá de Henares University. Spain

management administration

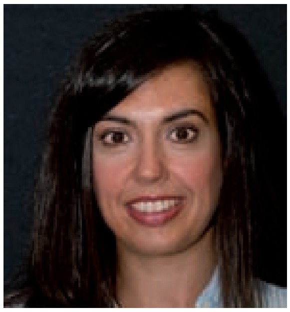
Dr. Covadonga Rosado

Manager



Miguel Ángel Rodiel

Technology Manager



Vanessa Fernández

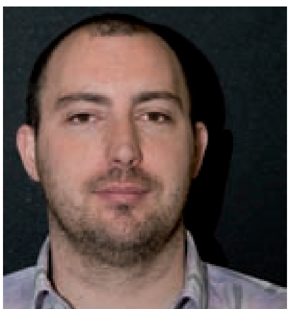
Personnel Manager

Eduardo Ciudad-Real

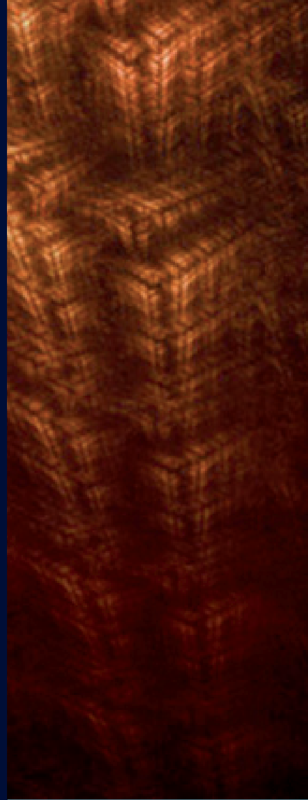
Accountant Assistant

Inés Leiva

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

- **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 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

- **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 500 ºC. 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-world 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 725 ºC. Equipped with Tzero technology, it provides flattest/reproducible baselines, superior sensitivity and resolution. It is also coupled with a refrigerated cooling system to operate over a temperature range of - 40 to 400 ºC and higher cooling rates of ~50 ºC/min.

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

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

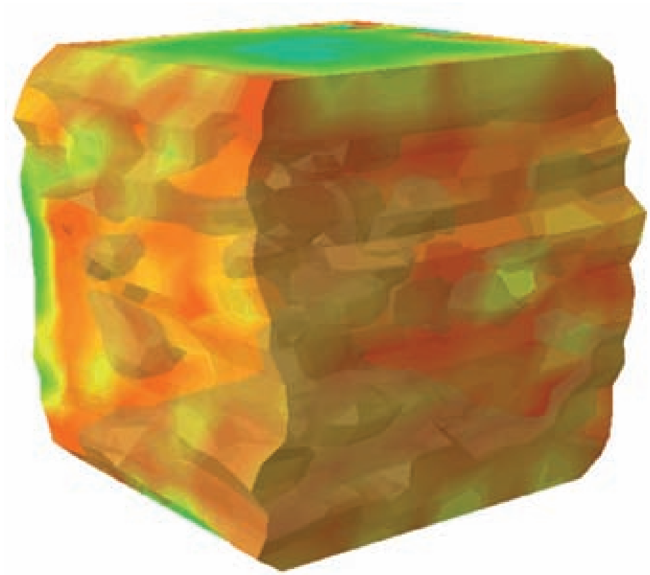
5.5. Simulation

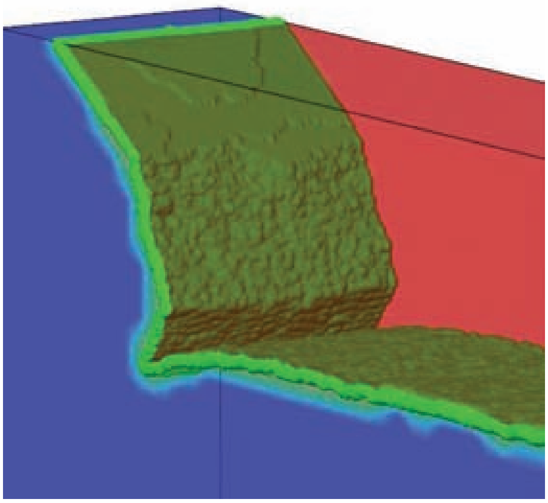
- **High Performance Computing Cluster** (60 cores, AMD Opteron 2356 & 2431)

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

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

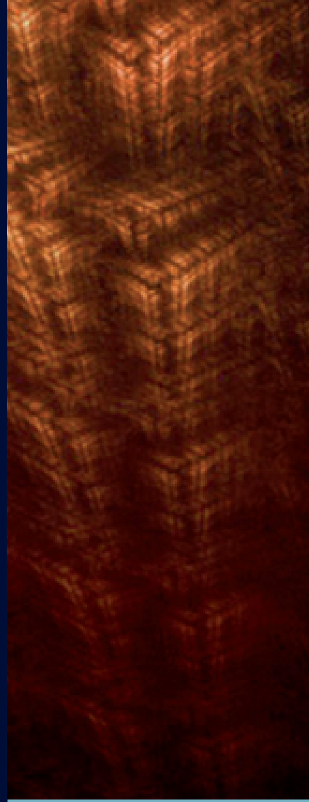
- Standard simulation, preprocessing and postprocessing programs (Abaqus, Hypermesh, Tecplot, etc.) as well as in-house developed codes for modelling and simulation of the mechanical behaviour and damage evolution of structural materials.





6

research projects



IMDEA Materials Institute currently participates in 21 research projects funded by industry, the European Unión, the Spanish Ministry of Science and Innovation, the Spanish Centre for Technological and Industrial Development (CDTI), and the Regional government of Madrid. A brief overview of some selected projects funded in 2010 is provided below:

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 / Dr. A. Dasari**

This large collaborative project aims to combine carbon nanotubes with high-performance carbon fibres to create highly innovative materials with tailored localization and orientation at both the nano and micro-scales in the final CFRP composite part, together with innovative production processes, which are capable of delivering high-end multifunctional structural parts, in a flexible and economically viable way. The structural parts developed during the course of the project need, obviously, to fit with the requirements of the main aerospace, train and automotive manufactures.

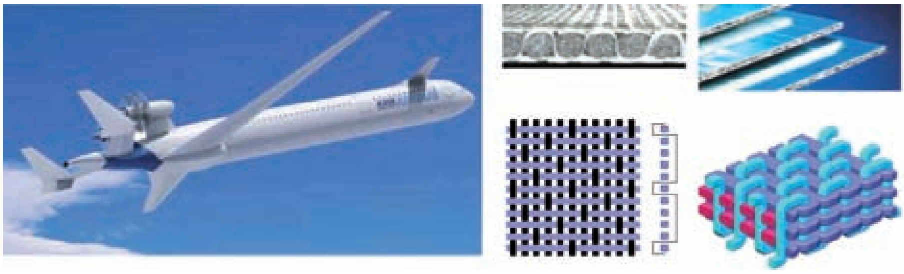
IMDEA Materials Institute contribution to the project includes the development of methodologies to model electrical conductivity and lightning impact performance for hierarchical nano-engineered fibre-reinforced composites and the evaluation of fire resistance.

ICE SHEDDING

"Design of advanced shields against high-velocity ice impact"

Funding: **Airbus Operations**
Duration: **2010-2011**
Principal Investigator: **Dr. C. González**

Industrial contract to design, manufacture, and validate innovative composite shields against high velocity ice impact for the new A30X next generation aircraft. The research activities include the design and manufacturing of new multifunctional and multimaterials shield coupons and panels for demonstration. The impact behaviour of the materials was experimentally validated against high-velocity impact of ice slabs at the Carlos III University and damage during impact was assessed using non-destructive evaluation techniques (ultrasounds and X-ray microtomography). Design optimization and validation to meet weight and thickness constraints is carried out by means of advanced numerical simulations carried out using the state-of-the-art virtual testing methodologies developed by IMDEA Materials Institute.



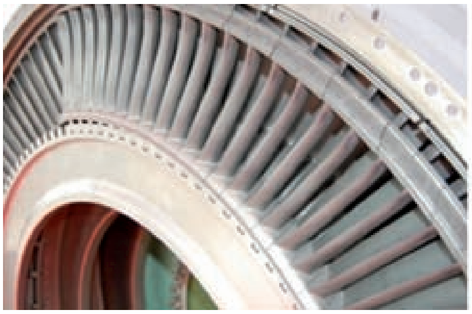
ALTIVA

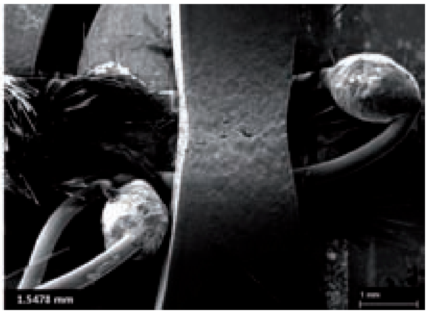
"Development of advanced gamma TiAl alloys for components with high reliability: microstructure design and modelling of the mechanical behaviour"

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**

Gamma-titanium aluminides are important intermetallic alloys targeted for high temperature aerospace applications in low pressure turbines (LPT) because they can provide increased thrust-to-weight ratios and improved efficiency. LPT materials must operate in aggressive environments at temperatures up to 800°C, and gamma titanium aluminides are projected to replace the heavier Ni-base superalloys currently being used.

In a first phase of the project, the deformation and fracture mechanisms of gamma TiAl samples fabricated by centrifugal casting have been investigated *in situ* by means of mechanical tests in a scanning electron microscope. This device allows analyzing in real time the mechanisms operative in different conditions of temperature and strain rate. Thus, it renders very valuable information regarding the kinetics of all these mechanisms, a difficult task to accomplish using ex situ observations. It has been found colony boundaries play a major role during deformation and fracture of gamma TiAl. A second phase of the work will involve exploring innovative processing routes in order to engineer advanced microstructures with an enhanced mechanical behaviour during creep at the service temperatures. Investigations will be performed using optical, transmission and scanning electron microscopy as well as texture analysis. The mechanical behaviour of the processed samples will be studied experimentally at room and high temperatures. The proposed basic research program will, finally, build quantitative models between microstructure, strength, ductility, and creep performance of gamma-titanium aluminide alloys.



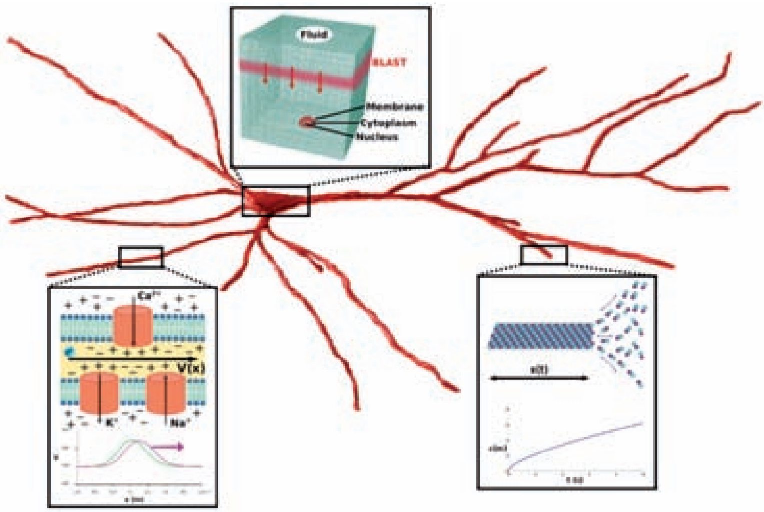


CAJAL BLUE BRAIN

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**

The Cajal Blue Brain Project (CajalBBP) is the Spanish participation within the International Blue Brain Project (BBP) which aims at reconstructing the brain piece by piece and building a virtual brain in a supercomputer. Different research groups and laboratories from Spanish institutions take part in this initiative, grouping together a large number of scientist, engineers and practitioners.

Participation of IMDEA Materials Institute in the project is focused on the electromechanical coupling within the different structures of the neuronal cell and on the structural evolution (mainly protein related) during the growth and migration of a neuron. These projects, in collaboration with medical and biological communities, and in synergy with de Cajal Blue Brain project´s goals, aim at bringing new simulation tools to the study of brain disease either due to sudden changes in the mechanical properties of the neurons (e.g. TBI) or to slowly evolving dysfunctions (e.g. Alzheimer or Huntington diseases).



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 / Dr. I. Sabirov**

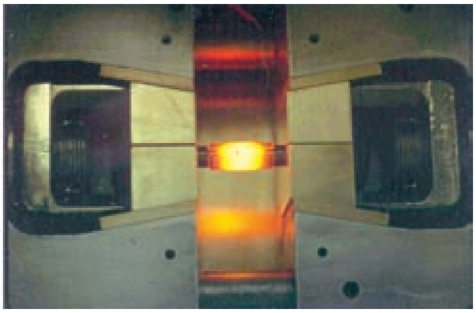
SEVENTH FRAMEWORK PROGRAMME

MATERA

Nozzle guide vanes (NGV) play a critical role in the thermodynamic efficiency, aerodynamic performance, and cost of ownership of gas-turbine engines. The objective of the VANCAST project is to develop the next generation of Ni-based superalloy nozzle guide vane design and manufacturing capability for low pressure turbines of advanced aircraft engines. The industrial benefits for the aviation industry of new NGV designs include reduced emissions, and improved fuel efficiency, reduced weight, and lower operating costs.

The new design and manufacturing capabilities will be established by building an improved modelling capability to simulate mold filling, solidification, residual stress and microstructure evolution during equiaxed casting processes. Critical DOE casting trials will be used to validate the model and enhance the manufacturing capability. These NGV designs and casting technologies will be evaluated using a combination of optimization studies using the enhanced software code developed in the present program, and the casting trials and analyses that will be performed.

IMDEA Materials Institute besides being in charge of the scientific/technical coordination of the project is responsible of studding the relationship between solidification history and microstructure, critical for the appropriate simulation of the casting process. This task is being carried out using the Gleeble 3800 system, which is the state-of-the-art technology to study the microstructural development of metallic alloys upon solidification.



SIMUCOMP

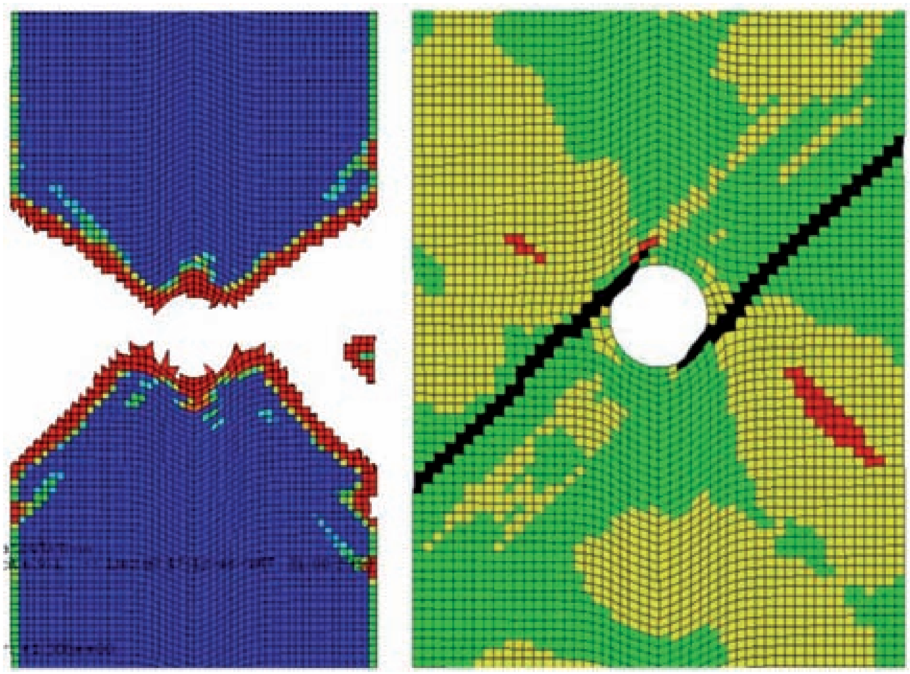
"Advanced numerical simulations of inter- and intralaminar failures in composite"

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**

The strategic objective of SimuComp is to help design and stress engineers assess the structural integrity and the damage tolerance of lightweight composite structures through provision of new accurate and predictive multi-scale failure models combined with original and computationally efficient novel numerical methods.

SimuComp is thus motivated by both industry needs (manufacturers: life prediction models; software vendors: efficient and predictive numerical solutions for damage and failure) and scientific advances beyond the current state-of-the-art as tackled by the project. The structures thus targeted will be based on multi-layered unidirectional composites as a demonstration of the accuracy of the new methods. The outcomes of the project will provide the industries with an easy-to-use set of numerical tools, able to predict multiple mode failure, at a level not yet achieved by current commercial FE software. Such drastic innovation will ultimately participate in designing lighter and stronger composites for the transportation and construction industry (especially for the aeronautical industry).

IMDEA Materials Institute is in charge of the overall scientific/technical coordination of the project and is responsible for the implementation in a large scale parallel computing code (such as Alya, in collaboration with the BSC) of state-of-the-art numerical methods for fracture initiation and propagation in UD composites materials. This includes advanced techniques such as XFEM and Discontinuous Galerkin method.



Other research projects currently running at IMDEA Materials Institute are:

"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: **2010-2011**
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")

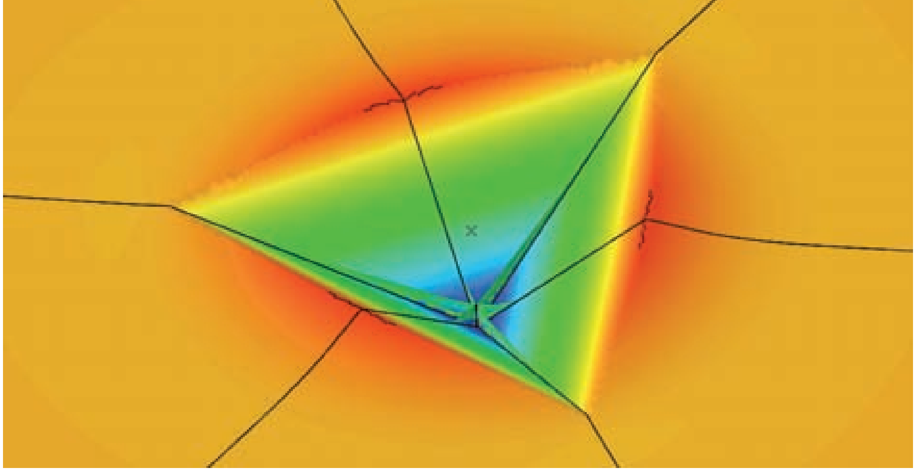
Funding: **Spanish Ministry of Science and Innovation**, **CDTI (CENIT Programme)**
Partners: National consortium led by Boeing Research, IMDEA Materials Institute collaborates with Aernnova Engineering Solutions Ibérica and Aries Complex Aeronáutica
Duration: **2010-2012**
Principal Investigator: **Dr. 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), 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: Polytechnic University of Madrid
Duration: **2010-2012**
Principal Investigator: **Dr. J. M. Molina-Aldareguía**



3D-CharMat ("3-Dimensional characterization of materials")

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

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

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

MORPHING ("Morphing materials for aeronautic applications")

Funding: **Regional Government of Madrid, IMADE (PIE Programme) and Aernnova Engineering Solutions Ibérica**
Partners: Aernnova Engineering Solutions Ibérica and IMDEA Materials Institute
Duration: **2009-2010**
Principal Investigator: **Dr. J. Segurado**

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, Europesn 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: **Spanish Ministry of Science and Innovation, CDTI (CENIT Programme)**

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 2008) 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**

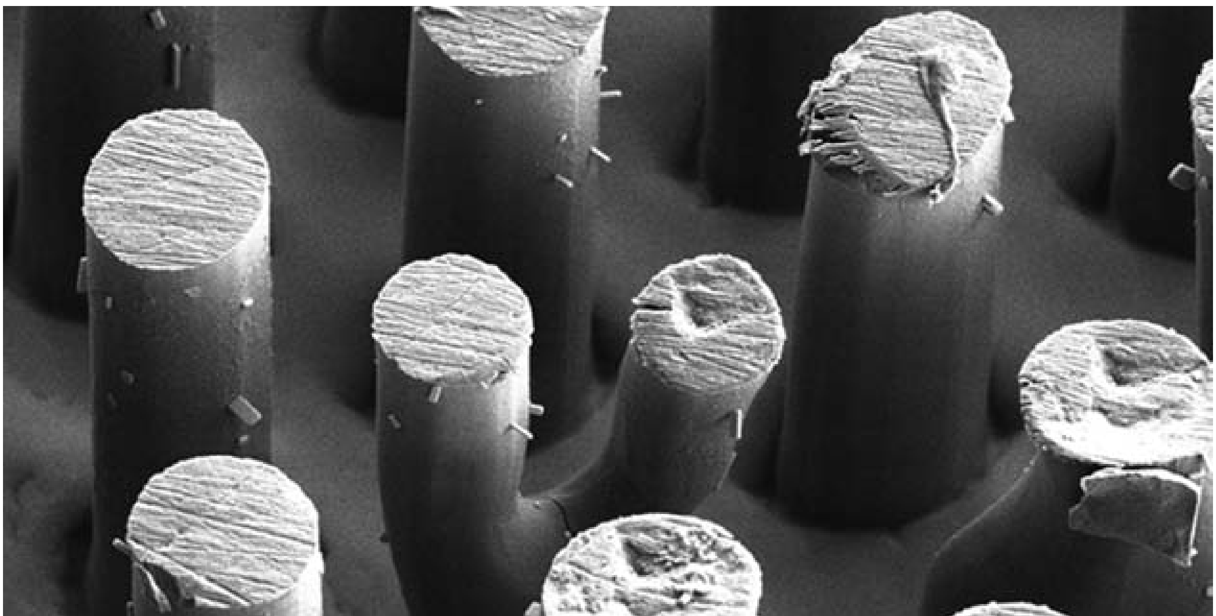
MAGNO ("Magnesium new technological opportunities")

Funding: **Spanish Ministry of Science and Innovation, CDTI (CENIT Programme)**

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

Duration: **2008-2012**

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



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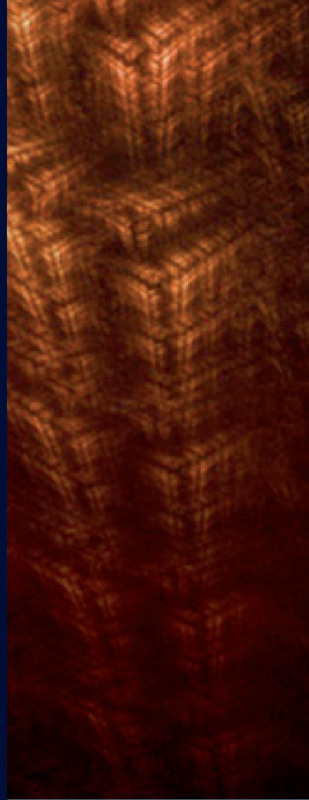
dissemination results



7.1. Publications

1. A. Dasari, G. Cai, Z.-Z. Yu, Y.-W. Mai. *"Flame retardancy of polymer-clay nanocomposites"*, in **Physical Properties of Polymer Nanocomposites** (Editors: S.C. Tjong, Y.-W. Mai) Woodhead Publishing Ltd., Cambridge, 2010.

2. A. Dasari, Z.Z. Yu, Q. X. Zhang, Y.-W. Mai. *"Toughening polypropylene and its nanocomposites with submicrometer voids"*. **Macromolecules 43**, 5734-5739, 2010.

3. A. Enfedaque, J. M. Molina-Aldareguía, F. Gálvez, C. González, J. LLorca. *"Effect of glass-fiber hybridization on the behavior under impact of woven carbon fiber/epoxy laminates"*. **Journal of Composite Materials 44**, 3051-3068, 2010.

4. A. García-Etxarri, J. Aizpurua, J. Molina-Aldareguia, R. Marcilla, J. Pomposo, D. Mecerreyes. *"Chemical sensing based on the plasmonic response of nanoparticle aggregation: Anion sensing in nanoparticles stabilized by amino-functional ionic liquid, Front"*. **Frontiers of Physics 5**, 330-336, 2010.

5. A. Mortensen, J. LLorca. *"Metal matrix composites"*. **Annual Review of Materials Research 40**, 407-410, 2010.

6. A. Ridruejo, C. González, J. LLorca. *"Damage micromechanisms and notch sensitivity of glass-fiber non-woven felts: an experimental and numerical study"*. **Journal of the Mechanics and Physics of Solids 58**, 1628-1645, 2010.

7. A. P. Zhilyaev, A. Sharafutdinov, M. T. Pérez-Prado. *"Phase transformations during high pressure torsion of pure Zr and of a Zr-2.5%Nb alloy"*. **Advanced Engineering Materials 12**, 754-757, 2010.

8. A.P. Zhilyaev, F. Gálvez, A. Sharafutdinov, M. T. Pérez-Prado. *"Influence of the high pressure torsion die geometry on the allotropic phase transformations in pure Zr"*. **Materials Science and Engineering A 527**, 16-17, 2010.

9. D. Marcos-Gómez, J. Ching-Lloyd, M. R. Elizalde, W .J. Clegg, J. M. Molina-Aldareguia. *"Predicting the thermal conductivity of composite materials with imperfect interfaces"*. **Composites Science and Technology 70**, 2276-2283, 2010.

10. E. Totry, J. M. Molina-Aldareguia, C. González, J. LLorca. "*Effect of fiber, matrix and interface properties on the in-plane shear deformation of carbon-fiber reinforced composites"*. **Composites Science and Technology 70**, 970-980, 2010.

11. F. Sket, K. Dzieciol, A. Borbély, A. R. Kaysser-Pyzalla, K. Maile, R. Scheck. "Microtomographic investigation of damage in E911 steel after long term creep". **Materials Science and Engineering A 528**, 103-111, 2010.

12. F. Sket, K. Dzieciol, A. Isaac, A. Borbély, A. R. Pyzalla. *"Tomographic method for evaluation of apparent activation energy of steady-state creep"*. **Material Science and Engineering A**, 527, 2112-2120, 2010.

13. G. P. Cai, A. Dasari, Z.-Z. Yu, X. S. Du, S .C. Dai, Y.-W. Mai, J. Wang. *"Fire response of polyamide 6 with layered and fibrillar nanofillers"*. **Polymer Degradation and Stability 95**, 845-851, 2010.

14. I. Sabirov, M. T. Perez-Prado, M. Murashkin, J. M. Molina-Aldareguia, E. V. Bobruk, N. F. Yunusova, R. Z. Valiev. *"Application of equal channel angular pressing with parallel channels for grain refinement in Aluminium alloys and its effect on deformation behaviour"*. **International Journal of Material Forming 3**, 411-414, 2010.

15. I. Sabirov, O. Kolednik. *"Local and global measures of the fracture toughness of metal matrix composites"*. **Materials Science and Engineering A 527**, 3100-3110, 2010.

16. I. Sabirov, R. Z. Valiev, I. P. Semenova, R. Pippan. *"Effect of equal channel angular pressing on the fracture behavior of commercially pure titanium"*. **Metallurgical and Materials Transactions A 41**, 727-733, 2010.

17. I. Ulacia, N. V. Dudamell, F. Galvez, S. Yi, M. T. Pérez-Prado, I. Hurtado. *"Mechanical behavior and microstructural evolution of a Mg AZ31 sheet at dynamic strain rates"*. **Acta Materialia 58**, 2988-2998, 2010.

18. J. Segurado, J. LLorca. *"Discrete dislocation dynamics analysis of the effect of lattice orientation on void growth in single crystals"*. **International Journal of Plasticity 26**, 806-819, 2010.

19. J. Tamayo-Ariztondo, J. M. Córdoba, M. Odén, J. M. Molina-Aldareguia, M. R. Elizalde. *"Effect of heat treatment of carbon nanofibres on electroless copper deposition"*. **Composites Science and Technology 70**, 2269-2275, 2010.

20. J. M. Contreras, A. Jimenez-Morales, J. M. Torralba. *"Experimental and theoretical methods for optimal solids loading calculation in MIM feedstocks fabricated from powders with different particle characteristics"*. **Powder Metallurgy 53**, 34-40, 2010.

21. J. M. Molina-Aldareguia, M. R. Elizalde. *"Metal matrix composites reinforced with nanosize reinforcements"*. **Composites Science and Technology 70**, 2227, 2010.

22. J. M. Molina-Aldareguia, M. T. Pérez-Prado, R. Z. Valiev, I. P. Semenova, I. Sabirov. *"High strength ultra-fine grained Titanium produced via a novel SPD processing route"*. **International Journal of Material Forming 3**, 407-410, 2010.

23. J. M. Ullbrand, J. M. Córdoba, J. Tamayo-Ariztondo, M. R. Elizalde, M. Nygren, J. M. Molina-Aldareguia, M. Odén. *"Thermomechanical properties of copper-carbon nanofibre composites prepared by spark plasma sintering and hot pressing"*. **Composites Science and Technology 70**, 2263-2268, 2010.

24. M. Campos, J. Sicre-Artalejo, J. J. Muñoz, J. M. Torralba. *"Effect of austempering conditions on the microstructure and tensile properties of low alloyed sintered steel"*. **Metallurgical and Materials Transactions A 41**, 203-209, 2010.

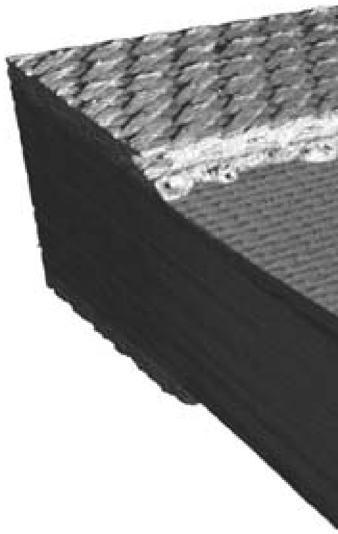
25. M. Multigner, S. Ferreira, E. Frutos, M. Jaafar, J. Ibáñez , P. Marín, M. T. Pérez-Prado, G. González-Doncel, A. Asenjo, J. L. González-Carrasco. *"Superficial severe plastic deformation of 316 LVM stainless steel through grit blasting: Effects on its microstructure and subsurface mechanical properties"*. **Surface & Coatings Technology 205**, 1830-1837, 2010.

26. M. J. Santofimia, T. Nguyen-Minh, L. Zhao, R. Petrov, I. Sabirov, J. Sietsma. *"New low carbon Q&P steels containing film-like intercritical ferrite"*. **Materials Science and Engineering A 527**, 6429-6439, 2010.

27. M.T. Pérez-Prado, A. Sharafutdinov, A. P. Zhilyaev. *"Thermal stability of pure bcc Zr fabricated by high pressure torsion Materials"*. **Materials Letters 64**, 211-214, 2010.

28. M. V. Aguirre, A. Martín, J. Y. Pastor, J. LLorca, M. A. Monge, R. Pareja. *"Mechanical behavior of Y2O3-doped W-Ti Alloys"*. **Journal of Nuclear Materials 404**, 203-209, 2010.

29. N. Stanford, I. Sabirov, G. Sha, A. La Fontaine, S. P. Ringer, M. R. Barnett. *"Effect of Al and Gd solutes on the strain rate sensitivity of magnesium alloys"*. **Metallurgical and Materials Transactions A 41**, 734-743, 2010.



30. S. H. Lim, A. Dasari, G. T. Wang, Z. Z. Yu, Y.-W. Mai, Q. Yuan, S. Liu, M. S. Yong. *"Impact fracture behaviour of nylon 6-based ternary nanocomposites"*. **Composites B 41**, 67-75, 2010.

31. R. Goel, A. Vechart, B. Schimizze, G. Christou, A. Jérusalem, L. R. Young, S. Son. *"Design of an advanced helmet liner to reduce TBI: simulations"*. **IMPLAST-SEM 2010 Fall Conference**, Providence, USA, 2010.

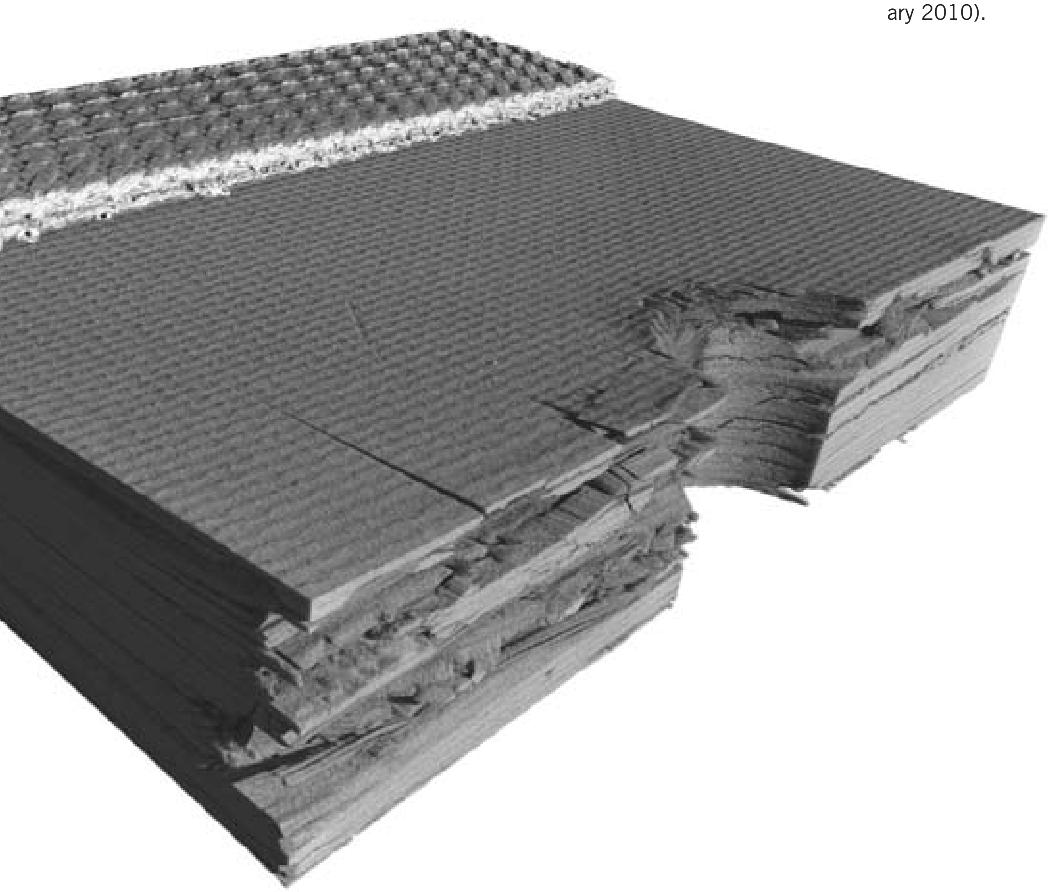
32. W. Li, R. Hu, Y.-W. Cui, H. Zhong, H. Chang, J. Li, L. Zhou. *"Computational study of atomic mobility for the bcc phase of the U–Pu–Zr ternary system"*. **Journal of Nuclear Materials 407**, 220-227, 2010.

7.2. Patents

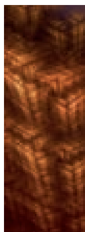
1. *"Method to design a synthetic fibres cable"*. C. González, J. M. Molina, K. Tamargo, J. LLorca. Application P201031862 (16 December 2010). Country: Spain. Joint ownership with Future Fibres rigging systems S.L.

2. "*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. Application P201001483 (19 November 2010). Country: Spain. Joint ownership with Future Fibres rigging systems S.L.

3. *"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. PCT/ES2010/070017 (15 January 2010).



patents



7.3. International Congresses

7.3.1. Invited and Plenary Talks

1. *"Thermal stability and mechanical behavior of nanostructured omega+beta Zr".* M. T. Pérez-Prado, A. P. Zhilyaev, I. Sabirov, G. González-Doncel, J. M. Molina-Aldareguía, B. Srinivasarao. **International symposium on Advances in Recrystallization and Processing of Fine Grained Materials** in honour of Prof. T. R. McNelley. Oñate, Spain, September 2010.

2. "*Anisotropy of mechanical properties in an ultra-fine grained pure Ti processed via a complex severe plastic deformation route*". I. Sabirov, M. T. Perez-Prado, J. M. Molina-Aldareguia, I. P. Semenova, G. Kh. Salimgareeva, R. Z. Valiev. **International symposium on Advances in Recrystallization and Processing of Fine Grained Materials** in honour of Prof. T. R. McNelley. Oñate, Spain, September 2010.

3. *"Computational modeling of deformation and fracture of non-woven felts"*. A. Ridruejo, C. González. J. LLorca. **IV European Conference on Computational Mechanics**. Paris, France, May 2010.

4. *"Deformation and failure mechanisms of fibre-reinforced composites by in-situ mechanical testing and computational micromechanics"*. J. M. Molina-Aldareguia, L. P. Canal, C. González, J. Segurado, J. LLorca. **International Symposium on Fine Scale Mechanical Characterization and Behavior (CAMTEC II)**. Cambridge, UK, March 2010.

5. *"Discrete dislocation dynamics simulations of void growth in FCC single crystals"*. J. LLorca, J. Segurado. **2nd International Symposium on Computational Mechanics of Polycrystals**. Bad Honnef, Germany, March 2010.

6. *"Fire response of polymer nanocomposite".* A. Dasari. **Symposium on Fire Protection Engineering in Railway Vehicles**. Madrid, Spain, September 2010.

7. *"On the quest of engineering ceramics for very high temperature structural applications"*. J. LLorca. **34th International Conference on Advanced Ceramics & Composites**. Daytona Beach, USA, January 2010.

8. *"Phase transformations in pure Zr by high pressure torsion"*. M. T. Pérez-Prado, A. P. Zhilyaev. **International Workshop on Atomic Transport in Bulk Nanostructured Materials and Related Unique Properties (ATBNM 2010)**. Rouen, France, May 2010.

9. *"Processing and thermomechanical properties of copper-carbon nanofibres composites for thermal management applications"*. J. M. Molina-Aldareguia. **12th International Ceramics Congress (CIMTEC 2010)**. Montecatini Terme, Italy, June 2010.

10. *"Virtual testing of composites. from materials to components"*. J. LLorca. **EADS Composite Technical Days**. Ottobrunn, Germany, October 2010.

11. *"Multiscale modeling of polycrystalline materials: a numerical implementation of the VPSC scheme into an implicit FE code"*. J. Segurado, R. Lebensohn, J. LLorca. **2nd International Symposium on Computational Mechanics of Polycrystals**. Bad Honnef, Germany, March 2010.

12. *"Thermoplastic elastomers: multiscale modeling, microstructure evolution and macroscopic instabilities"*. P. Ponte-Castañeda, O. Lopez, V. Racherla. **4th European Conference on Computational Mechanics**. Paris, France, May 2010.

invited and plenary talks

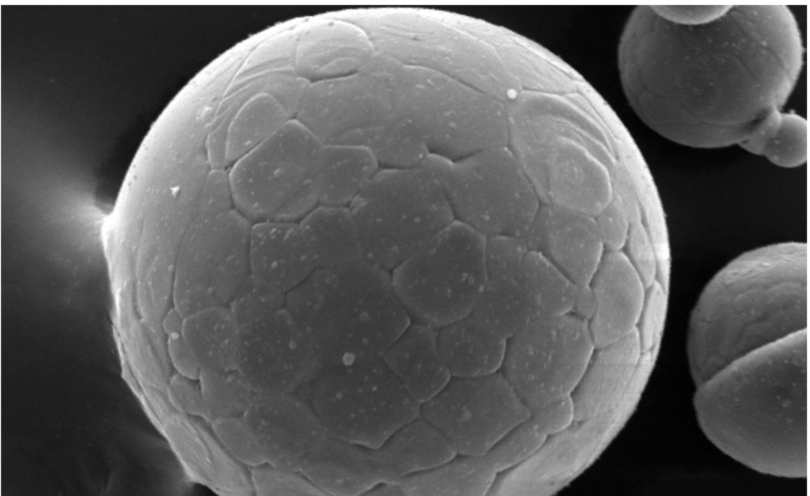
13. *"Bounds and estimates for nonlinear composites".* P. Ponte-Castañeda. **C.N.R.S. Summer School on Bridging of Scales in Mechanics of Materials**. Briançon, France, August 2010.

14. *"Variational linear comparison bounds for nonlinear composites with anisotropic phases".* P. Ponte-Castañeda. **International Workshop on Heterogeneous Materials and Composites** in honor of André Zaoui. Briançon, September 2010.

15. *"Nematic elastomers: macroscopic behavior and instabilities".* P. Ponte-Castañeda. **International Symposium on Stability and Nonlinear Solid Mechanics** in honor of Nguyen Quoc Son. Institut Poincaré, Paris, France, September 2010.

16. *"Simulations of decomposition kinetics of Fe-Cr solid solutions during thermal aging".* E. Martínez. **Solid-Solid Phase Transformations in Inorganic Materials**. Avignon, France, June 2010.

regular contributions



7.3.2. Regular Contributions

1. *"Texture evolution of AZ31 Magnesium alloy sheet at high strain rates".* I. Ulacia, S. Yi, M. T. Pérez-Prado, N. V. Dudamell, F. Gálvez, D. Letzig, I. Hurtado. **4th International Conference on High Speed Forming (ICHSF 2010)**. Columbus, USA, March 2010.

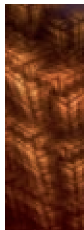
2. *"Nanostructuring of ultra-thin HfO2 layers for high-k/III-V device application".* M. Benedicto, J. V. Anguita, R. Alvaro, B. Galiana, J. M. Molina-Aldereguia, P. Tejedor. **11th International Workshop on Stress-Induced Phenomena in Metallization**. Dresden/Bad Schandau, Germany, April 2010.

3. *"Multi-Technique characterisation of MOVPE-Grown GaAs on Si".* C. S. Wong, N. S. Bennett, P. J. McNally, B. Galiana, P. Tejedor, M. Benedicto, J. M. Molina-Aldareguia, S. Monaghan, P. K. Hurley, K. Cherkaoui. **Spring Meeting E-MRS 2010**. Bordeaux, France, June 2010.

4. *"Study of kink band formation in PBO by bending tests of single filaments inside the SEM".* E. Lorenzo-Villafranca, K. Tamargo-Martínez, J. M. Molina-Aldareguia, C. González, J. LLorca. **Polymer Fibres 2010**. Edinburgh, UK, July 2010.

5. *"Damage evaluation of fiber reinforced polymers under impact".* F. Sket, J. M. Molina-Aldareguia, C. González, J. LLorca. **High-resolution CT X-Ray Symposium 2010**. Dresden, Germany, August-September 2010.

6. *"Application of equal channel angular pressing with parallel channels for grain refinement in Aluminium alloys and its effect on deformation behaviour".* I. Sabirov, M. T. Perez-Prado, M. Murashkin, J. M. Molina-Aldareguia, E. V. Bobruk, N. F. Yunusova, R. Z. Valiev. **13th International Conference on Material Forming (ESAFORM 2010)**. Brescia, Italy, April 2010.



7. *"High strength ultra-fine grained Titanium produced via a novel SPD processing route".* J. M. Molina-Aldareguia, M. T. Perez-Prado, R. Z. Valiev, I. P. Semenova, I. Sabirov. **13^{th} International Conference on Material Forming (ESAFORM 2010)**. Brescia, Italy, April 2010.

8. *"Mechanical and structural characterization of defects in CFRP materials".* M. Rodríguez?Hortalá, D. Salaberger, S. Hernández, H. P. Degischer. **Fachtagung Industrielle Computertomografie**. Wels, Austria, September 2010.

9. *"Rheological and thermal behavior of powder injection moulding (PIM) feedstocks fabricated with binder systems based on waxes".* J. Hidalgo, J. M. Contreras, B. Baile, A. Jiménez-Morales, J. M. Torralba. **Powder Metallurgy World Congress & Exhibition (PM2010)**. Florence, Italy, October 2010.

10. *"Fabrication of glass components by powder injection moulding (PIM) recycling glass waster".* J. Hidalgo, J. M. Contreras, D. Berzal, A. Jiménez-Morales, J. M. Torralba. **Powder Metallurgy World Congress & Exhibition (PM2010)**. Florence, Italy, October 2010.

11. *"Rheological behavior of powder injection moulding (PIM) feedstocks fabricated with a thermoplastic binder system based on polysaccharides".* J. Hidalgo, J. M. Contreras, S. González, A. Jiménez-Morales, J. M. Torralba. **Powder Metallurgy World Congress & Exhibition (PM2010)**. Florence, Italy, October 2010.

12. *"Production of sponge iron powder by reduction of by-products of the steelmaking industry"*. J. M. Torralba, M. E. Rabanal, M. I. Martin, F. A. Lopez. **World Congress on Powder Metallurgy (PM2010)**. Florence, Italy, October 2010.

13. *"Grain refining in sintered steels".* L. Fuentes, M. Campos, J. M. Torralba, A. Molinari. **World Congress on Powder Metallurgy (PM2010)**. Florence, Italy, October 2010.

14. *"Mechanical properties of PM Magnesium AZ91 alloy obtained by spark plasma sintering and extrusion"*. J. M. Torralba, J. M. Molina-Aldareguía, A. Gallego, A. P. Nogeira, G. Straffelini. **World Congress on Powder Metallurgy (PM2010)**. Florence, Italy, October 2010.

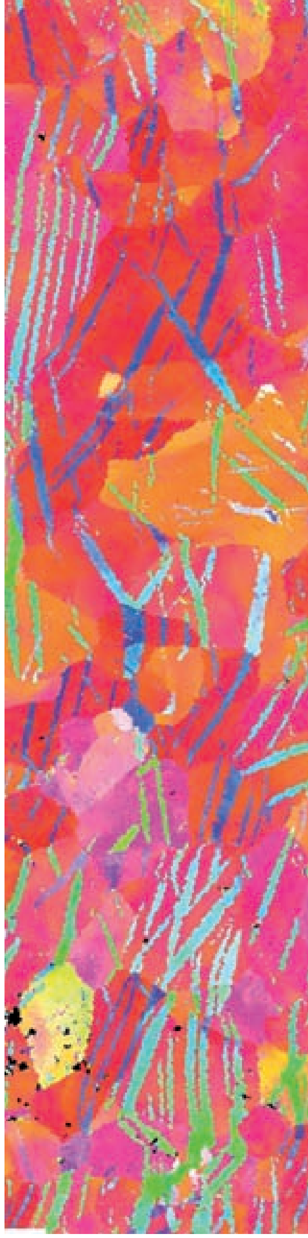
15. *"Microstructure and fracture behavior of high strength hybrid powder systems". P.* Shykula, E. Dudrova, R. Oro, J. M. Torralba, M. Campos, S. Bengtsson. **World Congress on Powder Metallurgy (PM2010)**. Florence, Italy, October 2010.

16. *"Atmosphere effects on liquid phase sintering of PM steels modified with master alloy additions". R.* Oro, M. Campos, J. M. Torralba, C. Gierl. **World Congress on Powder Metallurgy (PM2010)**. Florence, Italy, October 2010.

17. *"Void growth in polycrystals using 2D dislocation dynamics"*. J. Segurado, J. LLorca. **5^{th} International Conference on Multiscale Materials Modelling**. Freiburg, Germany, October 2010.

18. *"A finite element implementation of a polycrystalline material based on the viscoplastic self-consistent model"*. J. Segurado, R. Lebensohn, J. LLorca. **5^{th} International Conference on Multiscale Materials Modelling**. Freiburg, Germany, October 2010.

19. *"Micromechanics of polypropylene non-woven felts: experimental characterization and numerical modelling"*. A. Ridruejo, C. González, J. LLorca. **5^{th} International Conference on Multiscale Materials Modelling**. Freiburg, Germany, October 2010.



20. *"A model for complex deformation of polycrystalline materials based on the implementation of a viscoplastic self-consistent formulation in a FE implicit code".* J. Segurado, R. Lebensohn. **IV European Congress on Computational Mechanics (ECCM 2010)**. Paris, France. May 2010.

21. *"Some issues on fire response of polymer nanocomposites".* A. Dasari, Z. Z. Yu, Y.-W. Mai. **6th European Conference on Nanostructured Polymers Conference**. Madrid, Spain, April 2010.

22. *"Design of an advanced helmet liner to reduce TBI: simulations".* R. Goel, A. Vechart, B. Schimizze, G. Christou, A. Jérusalem, L. R. Young, S. Son. **SEM 2010 Fall Conference (IMPLAST 2010)**. Providence, USA, October 2010.

23. *"Ballistic testing of nanocrystalline hybrid plates".* J. Frontán, M. Dao, J. Lu, F. Galvez, A. Jérusalem. **International Symposium Failure and Damage Mechanisms of Armour Materials (LWAG 2010)**. Leganes, Spain, November 2010.

24. *"Ballistic properties of composites-nanocrystalline steel hybrid plates".* J. Frontán Vicente, F. Gálvez, J. Lu, M. Dao, A. Jérusalem. **International Symposium on Failure and Damage Mechanisms of Armour Materials (LWAG 2010)**. Leganes, Spain, November 2010.

invited seminars and lectures

7.4. Invited Seminars and Lectures

1. "Virtual testing of composites. From materials to components". J. LLorca. **Center for Composite Materials, University of Delaware**, Newark, USA, January 2010.

2. *"Computational materials engineering. An application of multiscale materials modelling".* J. LLorca. **École Nationale Supérieure des Mines**, St-Étienne, France, June 2010.

3. *"Computational materials engineering. An application of multiscale materials modelling".* J. LLorca. **Max-Planck Institute for Iron Research**, Dusseldorf, Germany, November 2010.

4. *"Computational modelling of deformation and fracture of non-woven felts".* C. González. **Department of Mechanical Engineering and Applied Mechanics. University of Pennsylvania**, Philadelphia, USA, October 2010.

5. *"Deformation of Mg alloys under dynamic conditions".* M. T. Pérez-Prado. **National Centre for Metallurgical Research (CENIM)**, Madrid, Spain, May 2010.

6. *"Experimental micromechanics of composite materials".* J. M. Molina-Aldareguia, L. P. Canal, C. González, J. Segurado, J. LLorca. Nanomechnics and Nanoindentation meeting, **NANOMEC Network. Civil Engineering School of Barcelona**, Spain, January 2010.

7. *"Fabrication of novel metallic phases by compression and shear".* M. T. Pérez-Prado. **Ceramic and Glass Research Institute-CSIC**, Madrid, Spain, May 2010.

8. *"High strength ultra-fine grained pure Ti processed via a novel SPD route".* I. Sabirov, M. T. Pérez-Prado, J. M. Molina-Aldareguia, I. P.

Semenova, G. Kh. Salimgareeva, R. Z. Valiev. **Missouri University of Science and Technology**, Rolla, USA, July 2010.

9. *"Plasticity at different length scales. Size effects and Dislocation Dynamics"*. J. Segurado. **Complutense University of Madrid**, Spain, March 2010.

10. "*Plasticity at the micro scale. Size effects and application to the void growth by Dislocation Dynamics"*. J. Segurado. **National Centre for Metallurgical Research (CENIM)**, Spain, March 2010.

11. *"Plasticity at the micro scale. Size effects and application to the void growth by Dislocation Dynamics"*. J. Segurado. **Polytechnic University of Madrid**, Spain 2010.

12. *"Where knowledge has no borders"*. A. Jérusalem. **European Commission EURAXESS Event**, Brussels, Belgium, October 2010.

7.5. Organization of Conferences, Workshops and Courses

1. International Summer School, European Powder Metallurgy Association. J. M. Torralba (Scientific and Academic Coordinator). Madrid, Spain, July 2010

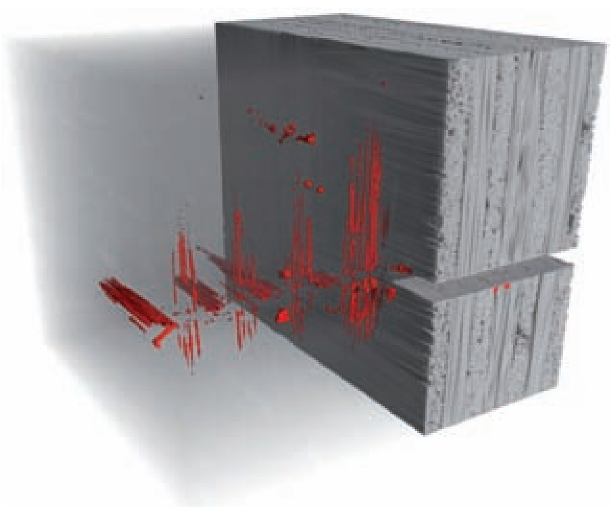
2. 3rd National Powder Metallurgy Congress. J. M. Torralba (Co-Chairman of the conference). Valencia, Spain, July 2010.

3. World Congress on Powder Metallurgy. J. M. Torralba (Technical Programme Committee). Florence, Italy, October 2010.

4. International Symposium on Advances in Recrystallization and Processing of Fine Grained Materials. M. T. Pérez-Prado (Member of the Organizing Committee). Oñate, Spain, September 2010.

5. 5th International Conference on Multiscale Materials Modelling. J. LLorca (Member of the International Advisory Board). Freiburg, Germany, October 2010.

6. 6th International Conference on Materials Structure & Micromechanics of Fracture. J. LLorca (Member of the International Advisory Board). Brno, Czech Republic, June 2010.



conferences
workshops
courses

seminars

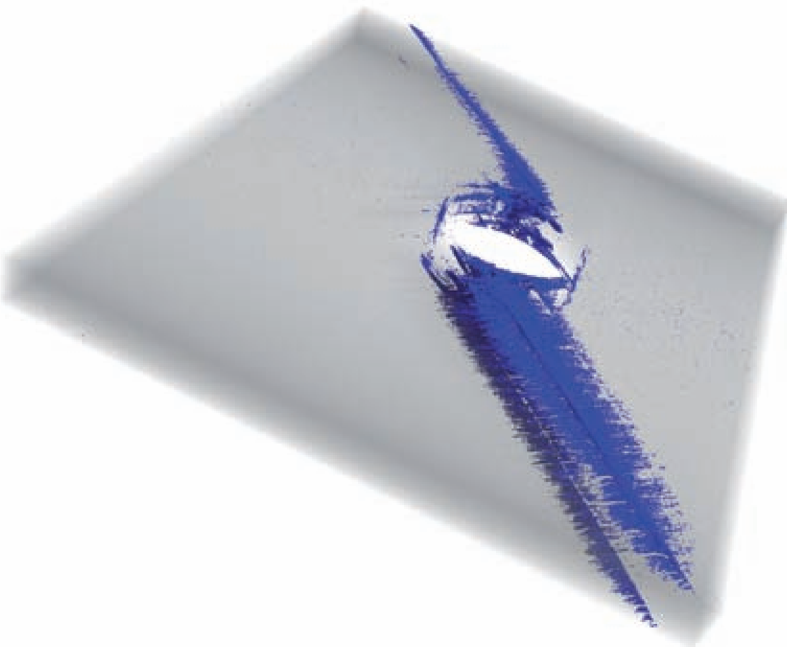
7.6. Seminars

1. *"Development of high-strength bimodally grained iron by mechanical alloying and spark plasma sintering".* **B. Srinivasa** (from National Institute for Materials Science, University of Rouen, Japan). February 2010.

2. *"Theoretical modelling of fast phase transitions in metallic materials".* **P. Galenko** (from Institute of Materials Science in Space R, German Aerospace Center, Germany). April 2010.

3. *"Directionally solidified eutectic alloys: from high temperature structural materials to functional nanodevices".* **S. Milenkovic** (from Institut für Chemische Technologie Anorganischer Stoffe, Johannes Kepler Universität, Austria). April 2010.

4. *"Non-conventional composite laminates: expanding the design envelope".* **P. P. Camanho** (from Department of Mechanical Engineering, University of Porto, Portugal). May 2010.



5. *"Electromechanical model of the heart".* **P. Lafortune** (from Barcelona Supercomputing Center, Spain). May 2010.

6. *"Computational thermo-kinetics, phase field modeling and their applications in alloy designs".* **Y. Cui** (from Department of Materials Science and Engineering, Ohio State University, USA). May 2010.

7. *"Light weight structural solutions".* **S. Saleem Khan** (from Institute for Materials Research, GKSS Research Centre Geesthacht GmbH, Germany). June 2010.

8. *"A synergistic multi-scale approach to damage in composite structures".* **R. Talreja** (from Department of Aerospace Engineering, Texas A&M University, USA). June 2010.

9. *"Variational principles for dissipative solids in physical and material space: implications to plasticity and fracture".* **C. Miehe** (from Universitat Stuttgart, Germany), June 2010.

10. *"Fundamental and practical evaluation of advanced surface treatments for light metals and alloys".* **E. Matykina** (from National Center for Metallurgical Research, *CSIC, Spain).* July 2010.

11. *"Towards material and structural virtual testing of laminates: micro / meso-modelling and associated computational challenges".* **O. Allix** (from *L.M.T.-Cachan, France). July 2010.*

12. *"From nano to macro: understanding materials through characterization at different length scales".* **G. Bruno** (from Corning Inc., USA). July 2010.

13. *"Design of advanced metallic materials by microstructure control*". **I. Gutiérrez** (from AIMEN Technology Center, Spain). September 2010.

14. *"Friction stir processing (FSP) of cast metals: processing – microstructure – property relationships".* **T. R. McNelley** (from Center for Materials Science and Engineering, Naval Postgraduate School, USA). September 2010.

15. *"Atomistic simulations for material science".* **I. Martin-Bragado** (from Synopsys Inc., USA). September 2010.

16. *"Electromagnetic materials measurement research".* **L. Kempel** (from Michigan State University, USA). October 2010.

17. *"Defect nanoengineering in graphene and nanotubes:* a new approach towards applications". **M. Terrones** (from Shinshu University, Japan). October 2010.

18. *"Textile materials in the form of performs, used for fibre reinforced composites*". **A. Rawal** (from Indian Institute of Technology Delhi, India). November 2010.

19. *"Multiscale modeling and microstructure-sensitive materials design".* **D. L. McDowell** (from Georgia Institute of Technology, USA), November 2010.

7.7. Fellowships

Marie Curie AMAROUT Incoming Fellowships, European Union-7th Framework Programme, 2010. **(Dr. F. Sket, Dr. B. Srinivasa-Rao, Dr. Y. Cui, Dr. R. Jerome, Dr. M. Agoras)**

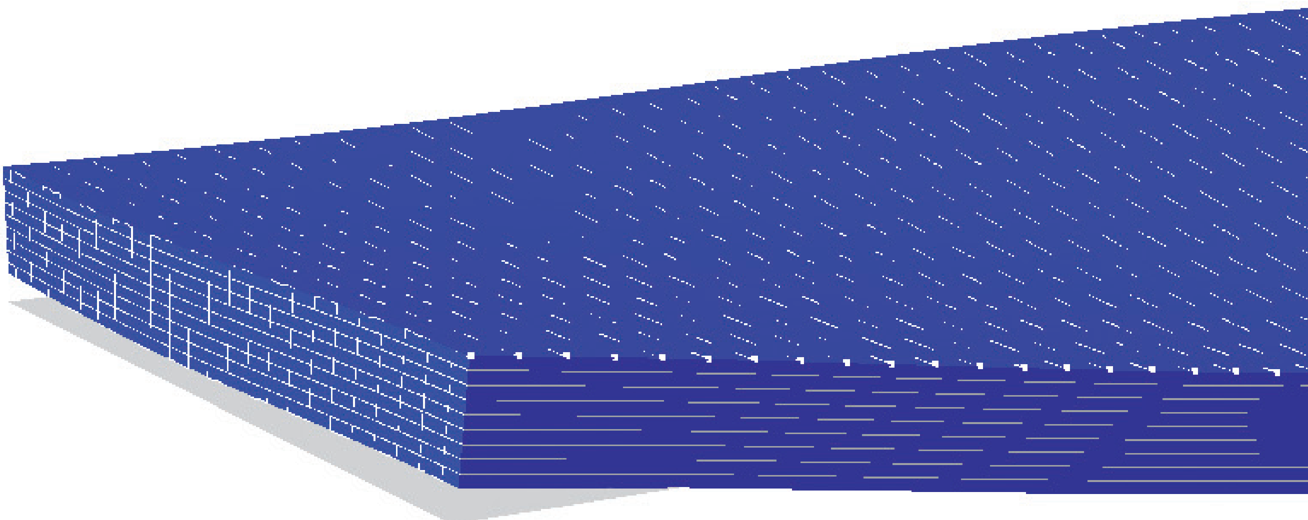
Ramon y Cajal Fellowships, Spanish Ministry of Science and Innovation, 2010 (**Dr. A. Dasari and Dr. S. Milenkovic**)

Juan de la Cierva Fellowships, Spanish Ministry of Science and Innovation, 2010 (**Dr. R. Seltzer**)

7.8. Awards

- **Dr. J. Segurado**. Young Investigator Award, Polytechnic University of Madrid (2010)

fellowships
awards



institutional activities

7.9. Institutional Activities

- Member of the Steering Committee of the *Spanish Technological Platform of Advanced Materials and Nanomaterials* (MATERPLAT)

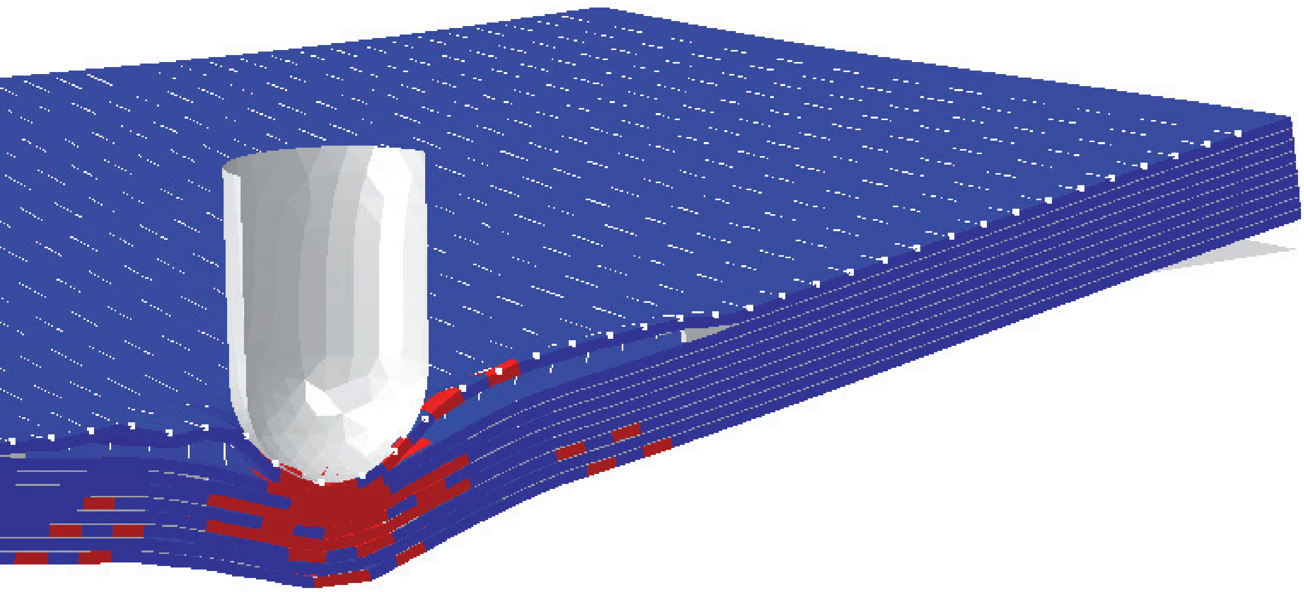
- Member of the Technological Clusters on Security and Renewable Energies promoted by *Instituto Madrileño para el Desarrollo* (IMADE)

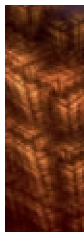
- Member of the Network of Research Laboratories of *Comunidad de Madrid* (REDLAB)

- Collaboration with the Department of Materials Science, Polytechnic University of Madrid to organize the *Materials Science Frontiers* Seminars

- J. LLorca was appointed Associate Editor of Composites Science and Technology, the leading international journal on composite materials published by Elsevier.

- Co-organizers of the Interuniversity Research Seminars Programme (A. D. Rosato, C. Miehe, D. L. McDowell)





7.10. Theses

theses

7.10.1. Advanced Studies Diplomas

"Mechanical behaviour of magnesium alloys at high strain rate"
Student: Nathamar Dudamell
Complutense University of Madrid
Advisors: Dr. M.T. Pérez-Prado and Dr. F. Galvez
Date: June 2010

"Optimization of the cure cycle of a composite materials processed by hot compression molding"
Student: Silvia Hernández
Polytechnic university of Madrid
Advisor: Dr. C. González
Date: June 2010

7.10.2. Master/Bachelor Theses

"Study of the deformation behaviour of the UFG Al alloy processed by ECAP-PC"
Student: Markel Bilbao
Polytechnic University of Madrid
Advisors: Dr. M. T. Pérez-Prado and Dr. I. Sabirov
Date: January 2010

"Evolution of the crystallographic texture during uniaxial deformation of a rolled sheet of the Mg alloy AZ31"
Student: Ana Fernández
Carlos III University of Madrid
Advisors: Dr. A. Jérusalem and Dr. M. T. Pérez-Prado
Date: May 2010

"Development of a helmet liner for protection against blast induced trauma"
Student: George Christou
Massachusetts Institute of Technology
Advisors: Dr. L. Young and Dr. A. Jérusalem
Date: June 2010

"Implementation and calibration of a rate-dependent crystal plasticity constitutive model for Magnesium alloy AZ31B"
Student: Julián García
Polytechnic University of Madrid
Advisor: Dr. A. Jérusalem
Date: July 2010

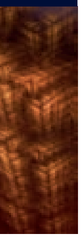
"Influence of the cold plasma treatments on the mechanical behaviour of the PBO HM fibre"
Student: Eduardo Lorenzo
Polytechnic University of Madrid
Advisors: Dr. J. M. Molina-Aldareguía and Dr. K. Tamargo
Date: July 2010

"Interfacial adhesion testing in polymer matrix composites"
Student: Genoveva Kelly
Polytechnic University of Madrid
Advisors: Dr. J. M. Molina-Aldareguía and M. Rodríguez
Date: July 2010

"Effect of the grain size and the temperature on the mechanical properties of an aluminum alloy"
Student: Eva Cristina Moreno
Carlos III University of Madrid
Advisors: Dr. I. Sabirov and M. T. Pérez-Prado
Date: September 2010

"Fire retardancy of PA6-based nanocomposites"
Student: Emeric Plancher
Ecole Nationale Superieure des Mines
Advisors: Dr. A. Dasari and Dr. B. Herrero
Date: September 2010

"Evolution of the properties of HPT processed Zr coupons"
Student: Bruno Romero



Polytechnic University of Madrid
Advisors: Dr. M. T. Pérez-Prado and Dr. F. Gálvez
Date: October 2010

"Fire properties of biodegradable polymer nanocomposites"
Student: Alfonso González
Complutense University of Madrid
Advisors: Dr. A. Dasari and Dr. B. Herrero
Date: October 2010

"Ballistic performance of nanocrystalline and nanotwinned ultrafine crystal steel"
Student: Jaime Frontán
Polytechnic University of Madrid
Advisors: Dr. A. Jérusalem and Dr. F. Gálvez
Date: October 2010

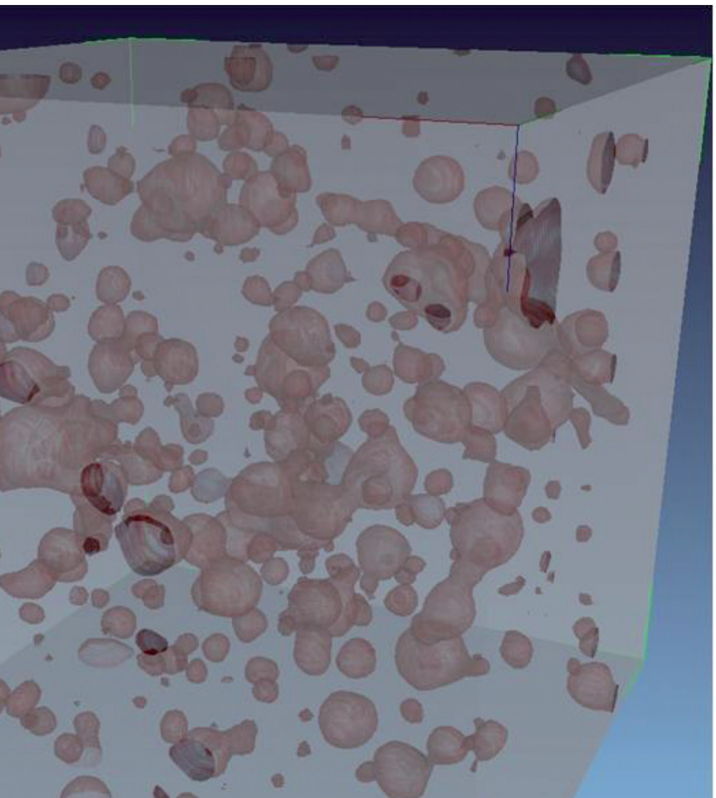
"Mechanical behaviour of magnesium alloys at high strain rate. Porosity analysis using X-ray computed tomography"
Student: Daniel Pamplona
Polytechnic University of Madrid
Advisors: Dr. F. Sket and N. Dudamell
Date: October 2010

7.11. Internships / Visiting Students

"Numerical modeling of nanocrystalline deformation"
Student: Vincent Péron Lührs
Universite de Liege
Advisors: Dr. Ludovic Noels and Dr. A. Jérusalem
Date: September 2010

"Effect of defects on composite materials"
Student: Michael Holzmeier
Technical University of Vienna
Advisors: Dr. J. M. Molina-Aldareguia and S. Hernández
Date: November 2010

"Development of electrospun ZrO2 coatings for improved biocompatibility"
Student: Armin Schmid
University of Bremen
Advisors: Dr. M. T. Pérez-Prado and Dr. A. Dasari
Date: December 2010



internships visiting students

7.12. Courses

"Materials for extreme working conditions"
Master on mechanical engineering and materials.
Polytechnic University of Valencia
Professor: Dr. M. T. Pérez-Prado

"Materials for microelectronics".
Máster on structural materials for new technologies.
University Carlos III of Madrid and University Rey Juan Carlos of Madrid
Professor: Dr. J. M. Molina-Aldareguia

"Structural materials for transport and energy technologies"
Master on structural materials for new technologies
Carlos III University of Madrid and Rey Juan Carlos University
Professor: Dr. J. M. Molina-Aldareguia

"Structural composites"
Master on structural engineering, foundations and materials
Polytechnic University of Madrid
Professor: Prof. J. LLorca, Dr. J. Segurado, Dr. C. González

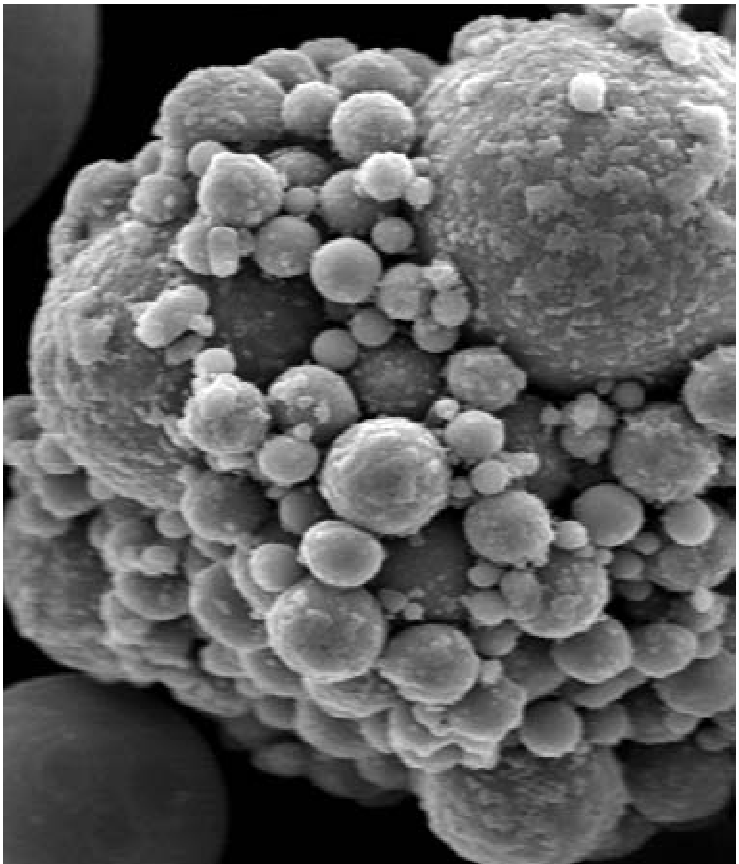
"Mechanics of composite materials"
Master on structural engineering, foundations and materials
Polytechnic University of Madrid
Professor: Prof. J. LLorca, Dr. J. Segurado, Dr. C. González

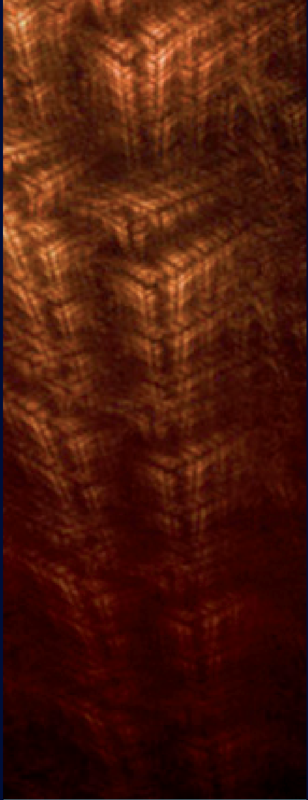
"Polymer nanocomposites: from transport to energy fields"
Master on structural materials for new technologies
Carlos III University of Madrid and Rey Juan Carlos University
Professor: Dr. A. Dasari

"Virtual testing strategies in composites and micro-macro scale relationships, multiscale modeling and related multifield problems"
IUTAM Summer School on modelling and simulation of multiscale continuum systems
International Center for Mechanical Sciences, Udine, Italy
Professor: Prof. J. LLorca

"Advanced simulation tools for composite materials: virtual testing"
Summer School on composite materials. New developments
Polytechnic University of Madrid
Professor: Dr. C. González

courses





8 scientific highlights

Put out the fire: designing the fire retardant polymer nanocomposites

'Fire' is an important topic, not just from a scientific viewpoint, but also from a day-to-day living perspective. Millions of fires every year leading to more than 300,000 deaths are reported world-wide and the direct property losses exceed €20 billion, according to the World Health Organization. As polymers form the core of the modern world and are reportedly a major contributor to fire incidents, understanding this science to fine-tune the materials for achieving highest fire safety standards is important. But conventional fire retardants, particularly halogen-based compounds are persistent organic pollutants of global concern and tend to generate corrosive and toxic combustion products like dioxins (polyhalogenated dibenzo-p-dioxins) and furans (polyhalogenated dibenzo-p-furans), severely affecting the eco-system in various ways.

Considering eco-friendliness, ultimate mechanical/ physical properties, and processing difficulties, unsatisfactory fire performance of polymer composites is a major obstacle. The incorporation of nanoscale fillers (like clays, carbon nanotubes, graphite oxide, POSS, etc) in polymers, though, showed a positive potential towards flame retardancy (reductions in heat release/mass loss rates and delayed burning, Fig. 1), they are unable to meet the existing fire standard requirements [1, 2]. This has led to the continued usage of conventional fire retardants (halogen/phosphorous based compounds or metal hydroxides).

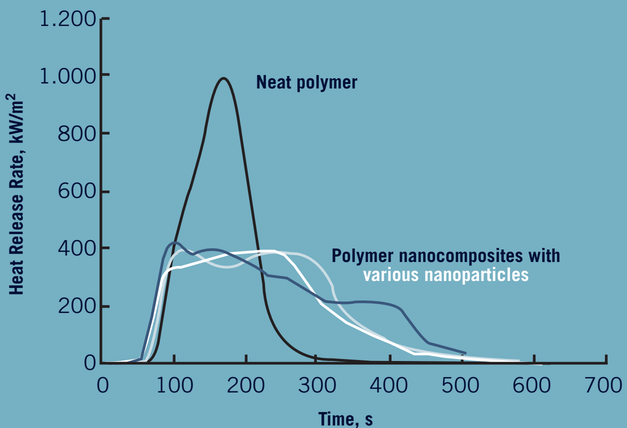


Figure 1. Significant reductions in heat release rates and delayed burning of polymer nanocomposites (with 5-10% loading of nanoparticles) compared to neat polymer.

designing the fire retardant polymer nanocomposites

Figure 2. Intumescent effect exhibited by a polymer nanocomposite without the addition of any conventional intumescent filler

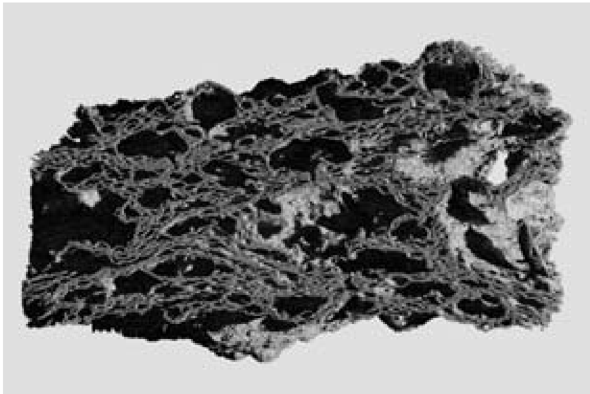


Figure 3. X-ray microtomogram of the combustion residue of a polymer nanocomposite

Emphasis of Multi-functional Nanocomposites group at IMDEA Materials Institute has been to achieve superior flame/smoke/toxicity performance in various polymers by designing and incorporating novel eco-friendly agents/nanoparticles (see for e.g. Fig. 2). Meticulous understanding (both qualitatively and quantitatively) of the steps involved in the combustion process of these materials allowed us to have an insight into the mechanisms of fire retardancy (Fig. 3), accurately delineate the boundary conditions and transport phenomena. In the process, issues with various processes occurring at sensitive stages of the combustion process have been identified that include thermal stability of the materials, homogeneity/uniformity of the barrier, char enhancement, and migration of nanoparticles to the burning surface. Addressing these issues will ultimately result in the development of the next generation of polymer nanocomposites which are eco-benign and exhibit superior flame retardancy with balanced mechanical properties.

[1] Dasari A. et al.. Roles of graphite oxide, clay and POSS during the combustion of polyamide 6. Polymer 50, 1577-1587, 2009

[2] Dasari A. et al.. Flame retardancy of highly filled polyamide 6/clay nanocomposites. Nanotechnology 18, 445602, 2007

Micromechanical testing in composites: the importance of the interface

the importance of the interface

Fibre reinforced polymers (FRP) are nowadays extensively used in applications where outstanding mechanical properties are necessary in combination with weight savings. Good examples can be found in the A380, the last civil Airbus aircraft containing up to 25% in weight of composite materials (used for wings, fuselage sections and tail surfaces) while the Boeing 787 Dreamliner claims to be the first airliner with a fully composite fuselage manufactured with advanced technologies. Despite all existing information and current knowledge about these materials, the accurate prediction of the failure stress of composite materials and structures has been an elusive problem because of the complexity of their failure micromechanisms. Of all them, fibre matrix debonding often dominates the composite failure, as shown in figure 1 for a crack growing in a glass reinforced polymer (GRP).

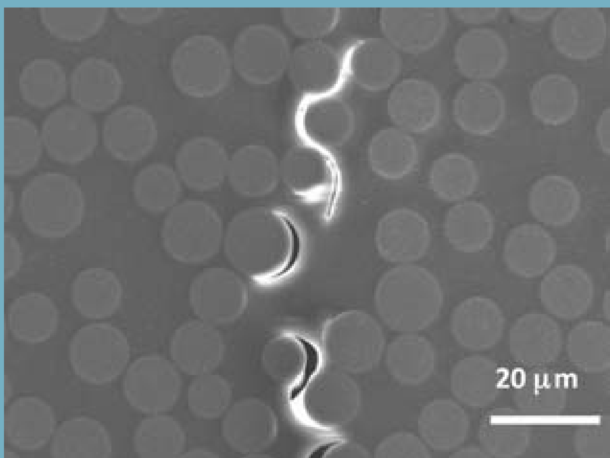


Figure 1. SEM image of a growing crack in a GRP highlighting the importance of the fibre debonding micromechanism.

A large effort is dedicated at IMDEA Materials Institute to develop novel micro and nanomechanical testing techniques to allow us for measuring the fibre-matrix interfacial strength with great accuracy. For instance, in the push-in technique, a single fibre is pushed with a flat punch on the cross-section of a bulk composite, as shown in figure 2. The interfacial strength can be extracted from the load at which debonding starts, as demonstrated by careful FE simulations (figure 3) [1]. The main advantage of the technique is that it can be employed in any composite material without extensive sample preparation. Alternatively, we also use the push out technique in which a very thin slice of the

(a) (b)

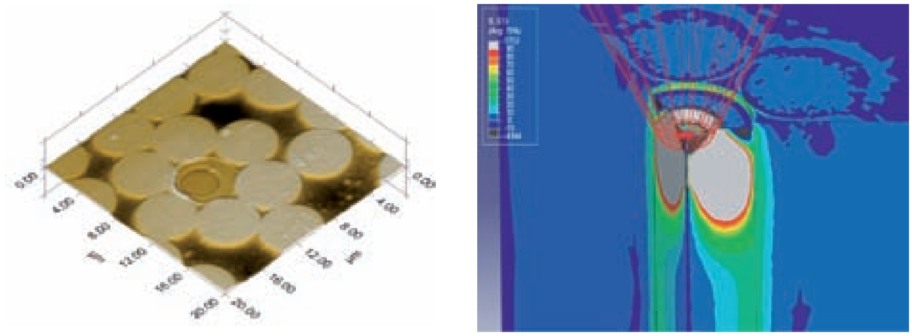


Figure 2. (a) AFM image of the pushed-in fibre in a CFR epoxy composite and (b) finite element simulation of the push-in tests showing the shear stresses at the fibre-matrix interface

material has to be prepared. In this case, sample preparation is cumbersome as the slice needs to be just a few micrometers in thickness but the interpretation is greatly facilitated, as full interfacial decohesion can be achieved by pushing the fibre and extracting it from the other side, as shown in figure 3.

(a) (b)

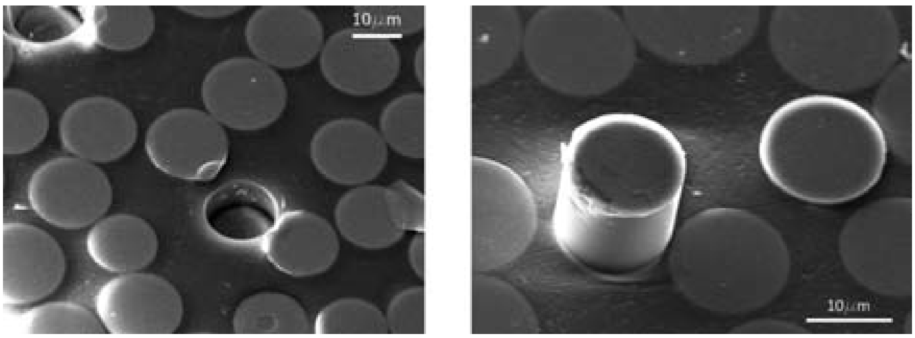


Figure 3. SEM image of the push-out test in a glass fibre composite: (a) front side and (b) back side showing the extraction of the pushed fibre.

The use of these techniques is putting IMDEA Materials Institute at the forefront of micromechanical testing in composites. This is the first step towards the development of full virtual testing methodologies in composites: once the composite constituent properties are experimentally determined at the microscale, they can be fed into computational micromechanical simulations to predict the macroscopic response of the material without the need of time consuming and expensive experimental campaigns.

[1] 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

improving the strenght of PBO fibres

Improving the compressive strength of PBO fibres

Poly p-(phenylene benzobisoxazole) or PBO fibres are the fibres of choice in high-performance applications where high strength and low weight are important, such as in competition yacht rigging (see figure 1). However, PBO fibres are highly anisotropic, which makes them relatively weak under axial compression, with a compressive strength one order of magnitude lower than in the tensile. This obviously limits the application of PBO fibres in structural components subjected to both tensile and compressive stresses or when axial compressive loads may appear during service.

Figure 1. PBO cables for yacht rigging applications.

In order to alleviate this limitation, a multidisciplinary research team of IMDEA Materials Institute has carried out careful fundamental studies of the compressive deformation of PBO fibres, by carrying out bending tests inside a Scanning Electron Microscope. These studies have shown that failure under compression is triggered at low strains by the initiation of a kink band from the surface by a shear instability, which propagates rapidly through the fibre cross-section to form a knuckle, as can be seen in the set of images of figure 2, taken at increasing bending strains. Under further compressive or tensile deformation, the strain is localized in the knuckle leading to a considerable reduction of the fibre tensile strength [1].

In order to alleviate the limitation of PBO fibres in compression, and based on these fundamental studies, the members of the team have been able to develop nitrogen plasma surface treatment (patent pending) to improve the mechanical behaviour of PBO fibres under axial compression. Specifically, the new surface treatment leads to a dramatic improvement (of the order of 40%) in the critical compressive strain for knuckle formation with a negligible effect on the tensile strength. This significant improvement opens a wide range of new possibilities for the use PBO fibres in advanced composite materials, ballistic protection textiles, structural cables, etc.

[1] E. Lorenzo, K. Tamargo, J. M. Molina-Aldareguia, C. González, A. Martínez, J. M. D. Tascón, M. Gracia, J. LLorca. Influence of plasma surface treatments on kink band formation in PBO fibres during compression, Journal of Applied Polymer Science (2011) in press.

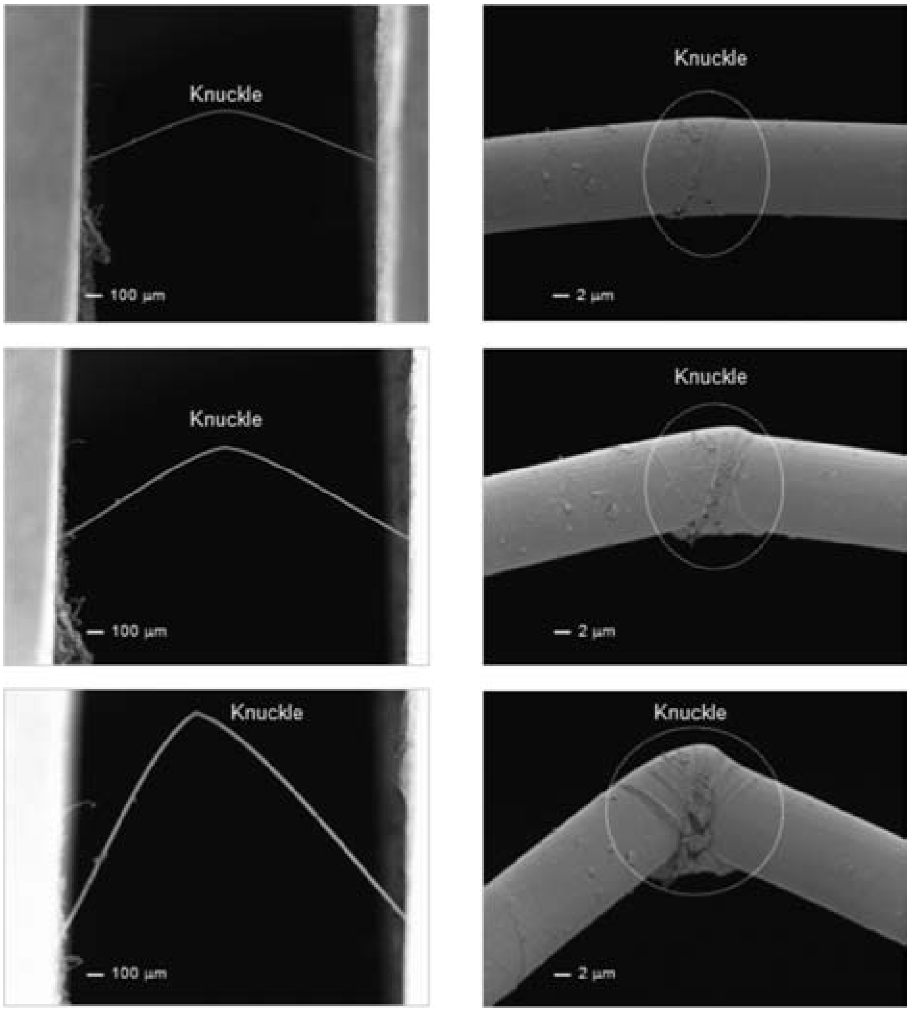
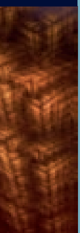


Figure 2. Kink band formation during the bending process of a PBO fiber, as seen during in-situ mechanical testing inside the SEM.



the effect of defe

The effect of defects in composites: X-Ray Computed Tomography

X-Ray computed tomography

Carbon fibre-reinforced polymer-matrix composites are nowadays extensively used in aeronautical applications due to their high specific stiffness and strength. In structural applications, manufacturing by autoclave is chosen because ensures a virtually defect free composite. However, autoclave manufacturing is expensive and new out-of-autoclave techniques are required to widespread the use of composites to other industrial sectors. For this reason, it is crucial that the effect of manufacturing defects in the mechanical properties of composites is better understood. IMDEA Materials Institute is currently focused on this subject using non-destructive analysis techniques, such as X-ray computed tomography (XCT). This technique is based on the computer-assisted reconstruction of three-dimensional microstructures of materials based on X-ray radiographies taken from various viewing angles. The development of new X-ray generation and detection techniques allow now to achieve sub-micrometer resolutions, making this technique a valuable tool for studying manufacturing defects and damage propagation in composites in great detail.

Figure 1 shows four identical carbon fibre reinforced composite panels that have been processed by hot-press using different curing cycles. The pores are highlighted in red and the results show that the curing cycle has a large effect on the void content, with laminate C-2 containing the least volume fraction of pores. Moreover, the technique allows extracting numerous conclusions about the formation of the pores (see [1]), that were not understood before. For instance, the voids tend to form channels that are always aligned with the fibre direction. The elongation and size distribution of these voids are indicative of two different void origins. The smaller ones, with more rounded shapes could come from internal voids within the prepreg, either present before the consolidation (gas bubbles from resin mixing operations, broken fibres) or generated by diffusion of water during the cure cycle. Long, elongated voids are the result of air entrapment and wrinkles created during lay-up. In addition, the results demonstrate that porosity is mainly concentrated in resin-rich regions, separated by a skeleton of fibre-rich zones. This peculiar distribution of the porosity within the laminate points to a process of inhomogeneous consolidation. These observations are very relevant from the viewpoint of understanding and simulating void formation, because most of the models for void nucleation and growth during curing of thermoset-based composites assume that voids develop within a homogenous medium. A team at IMDEA Materials Institute is currently working on more realistic models of void formation during resin curing to account for these observations.

[1] S. Hernández, F. Sket, J. M. Molina-Aldareguia, C. González, J. LLorca. Effect of curing cycle on void distribution and interlaminar shear strength in polymer-matrix composites, Composites Science and Technology, 71 (2011) in press.

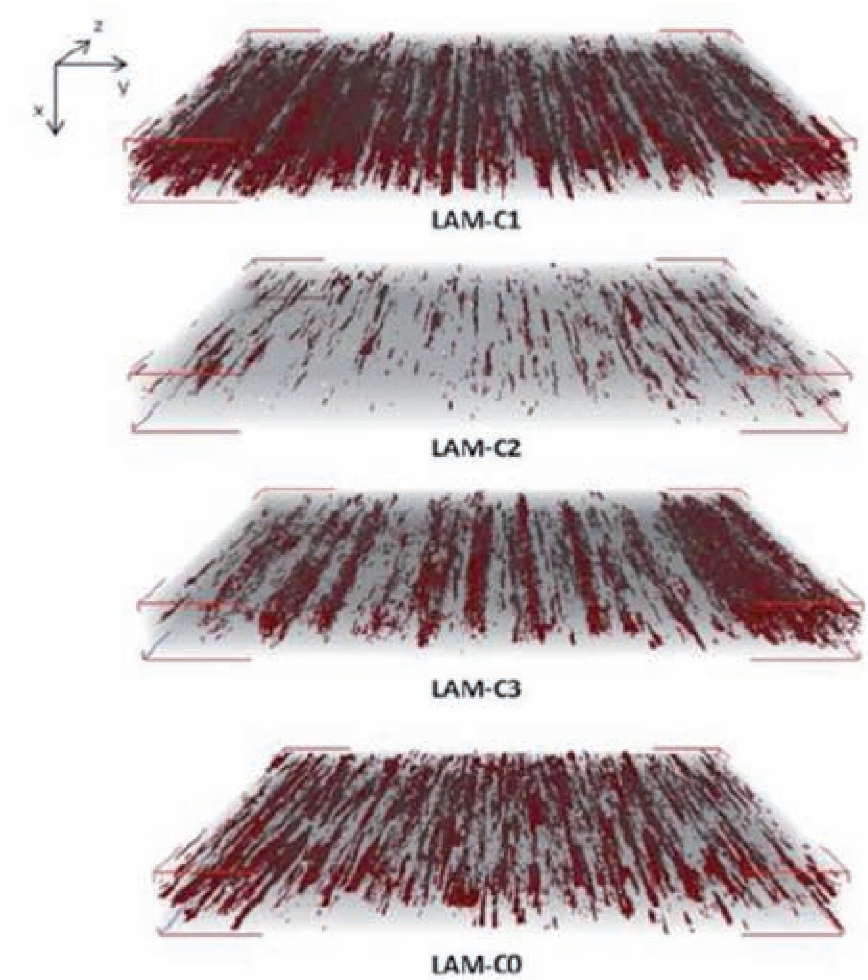


Figure 1. Tomography of identical carbon fibre unidirectional laminates subjected to different curing cycles. Porosity is highlighted in red showing the effect of the curing cycle on the final porosity, with laminate C2 containing the least volume fraction of pores.

watching m

Watching metals alive

Researchers at IMDEA materials Institute are investigating the in-situ deformation of metallic materials using a tensile testing micromachine coupled to a scanning electron microscope (Fig. 1a). This device allows to analyze in real time, the deformation, recrystallization and fracture mechanisms operative in these materials in different conditions of temperature and strain rate. Thus, it renders very valuable information regarding the kinetics of all these mechanisms, a difficult task to accomplish using ex-situ observations.

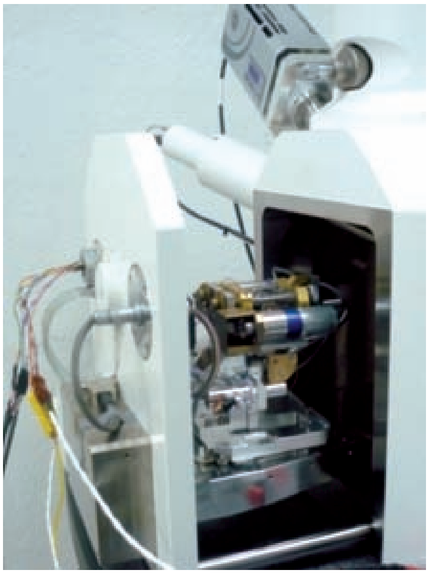
In particular, the in-situ deformation of magnesium alloys, very light metals that are increasingly being introduced in transportation vehicles, has been investigated at various temperatures. It has been concluded that grain boundary sliding, a mechanism consisting on the sliding of grains along its interfaces without significant deformation of the grain interiors, predominates at intermediate temperatures during quasi-static straining. At lower and higher temperatures, deformation is mostly controlled by crystallographic slip and twinning. Fig. 1b illustrates the surface of the AZ31 Mg alloy after deformation at 250°C. The white lines inside the grains are an indication of the presence of crystallographic slip. The waviness of the boundaries suggests, additionally, the presence of dynamic recrystallization.

The deformation and fracture mechanisms of gamma TiAl alloys, a promising material that is currently being used to build low pressure turbines for aircraft, have also been investigated using this technique. These materials are known for their high strength and low oxidation resistance, which makes them suitable for applications under extreme service conditions. It has been observed that, during creep at 700°C, colony sliding is a dominant mechanism during deformation. As a consequence, cracks nucleate at colony boundaries and then propagate along the colony interfaces until catastrophic failure ensues. Figures 2 a-c illustrate a sequence of crack nucleation and propagation. Thus, if the behaviour of these alloys under service conditions is to be optimized, special care must be taken in improving the resistance of colony boundaries to sliding.

[1] R. Muñoz-Moreno, E. M. Ruiz, M. T. Pérez-Prado, C. Boehlert. An in-situ SEM evaluation of the creep deformation behaviour of a gamma TiAl alloy. Aerodays 2011, Madrid.

etals alive

(a)



(b)

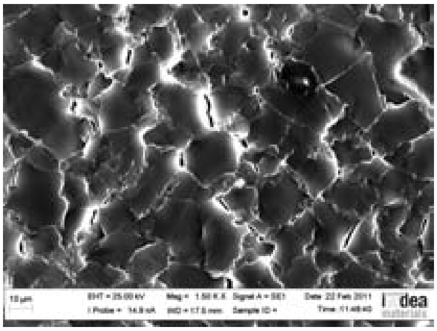


Fig. 1. (a) Tensile testing micromachine coupled to an scanning electron microscopy; (b) MgAZ31 alloy deformed at quasi-static strain rates at 250°C.

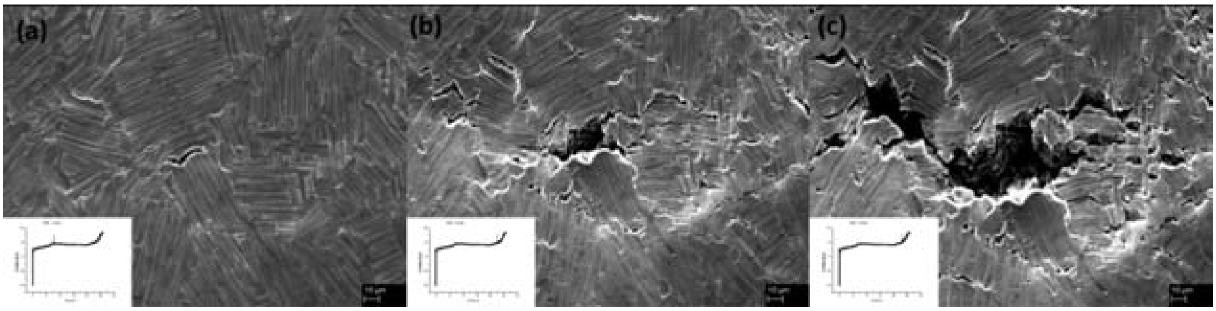


Fig. 2. Nucleation of a crack in a γTiAl alloy creep deformed at 700ºC and propagation of that crack along the colony boundaries with increasing testing time (a) 7.6h; (b) 22.4h; (c) 23.1h.

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