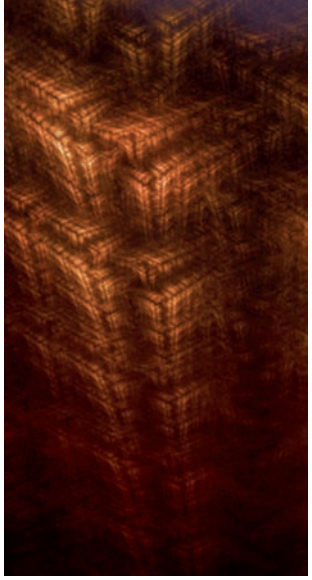

madrid institute
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IMdea
materials

annual report

foreword

foreword

Javier LLorca
Director, IMDEA Materials Institute
March 2013

annual report
2012

After wandering during a few years in provisional facilities, we have reached the promised land in 2012. Construction of the new building was completed in May and at the end of July all staff and equipment had moved to Getafe. The arrival was tough (only one elevator in operation, no air conditioning, etc.) but the enthusiasm overcame the logical difficulties of the first days. The new building was officially inaugurated on November 20th by Mr. Ignacio González, President of the Regional Government of Madrid.

The availability of the new building has been critical to expand our capacities with the construction and installation of new research infrastructures. In particular, furnaces for the processing of graphene, C nanotubes and CNT fibres were designed and built by the Institute scientists and are already supplying nanomaterials for different research projects. Our capabilities to manufacture advanced metallic alloys were enhanced with the acquisition of a system for vacuum induction melting and casting, while the nanomechanics laboratory become one of the world leaders in the area of high temperature nanomechanics with the installation of a new nanoindentor with high temperature capabilities (up to 750ºC) in an inert environment.

In addition, following the advice of the Scientific Council, we decided to organise the research activities of the institute along four research programs which cover the main thrusts areas in which the Institute is committed to become a world leader. They are devoted to

- Nanomaterials and Nanomechanics
- The Next Generation of Composite Materials
- Alloy Design, Processing and Development
- Integrated Computational Materials Engineering

These programs are focused on the development of advanced materials mainly in the sectors of transport, energy, information technology and manufacturing as well as on the exploration of emerging materials and processes for sustainable development.

Finally, IMDEA Materials Institute has continued growing during 2012 in terms of talented researchers, projects and scientific results. The research staff at the end the year has reached 65 researchers, while the project funding from industrial contracts and European projects increased by 51% and 60%, respectively, with respect to the previous year. In addition, 65 papers were published in peer-reviewed international journals (as compared with 36 in 2011) and the numbers of citations increased by almost a factor of 2 in comparison with 2011. All these figures (and many others that can be found in this Annual Report) show the ability of the Institute to fulfil its triple mission of attraction of talent, research of excellence and technology transfer to industry.

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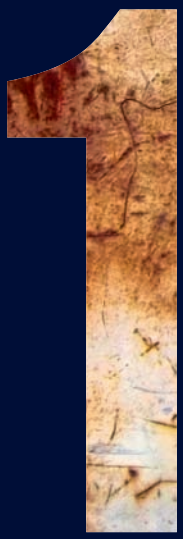

annual report 2012

1.1. About IMDEA Materials Institute

IMDEA Materials (Madrid Institute for Advanced Studies of Materials) is a non-profit independent research institute promoted by the Madrid regional government (Comunidad de Madrid) to perform research in Materials Science and Engineering. IMDEA Materials 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 to industry in a number of strategic areas (water, food, energy, materials, nanoscience, networks and software).

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

1.2. Appointments to the Board of Trustees and Scientific Council

- **Dr. Juan Ángel Botas,** Deputy General Director for Research of the Madrid Regional Government replaced to Dr. Jorge Sainz as one of the permanent trustees from the Comunidad de Madrid.
- **Prof. Ángel Arteaga Iriarte,** Director of the Eduardo Torroja Institute for Construction Science (CSIC) replaced Prof. Victor Ramón Velasco as one of the trustees from universities and public research institutions.

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

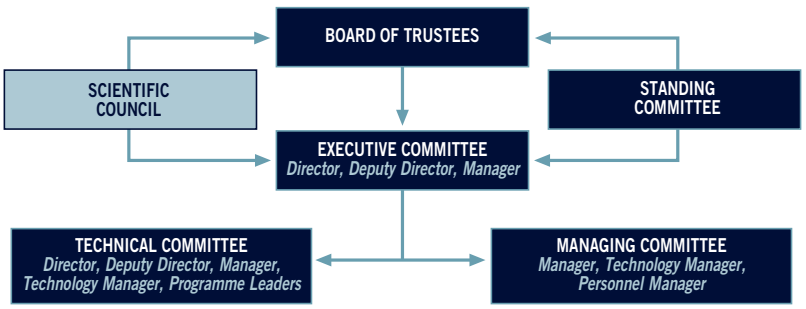

Figure 1. Organization chart of IMDEA Materials Institute

1.4. Inauguration of the Building

The construction of the building of IMDEA Materials Institute was finished on May 7th 2012. The institute building, with a surface of 9000 m^2, includes office space for management and researchers, laboratories (processing of nanomaterials and nanocomposites, processing of advanced structural materials, chemical and microstructural characterization, mechanical and thermal characterization, nanomechanics and computational materials engineering) as well as an open area to host conferences and scientific workshops.

Figure 2. IMDEA Materials Institute in Tecnogetafe.

The Institute personnel moved to the new building on July 23rd, once the permissions from the municipality were granted, and most of the scientific infrastructures were installed during July and August. The new building was officially inaugurated on November 20th by Mr. Ignacio González, President of the Regional Government of Madrid, who was accompanied by the Counsellor of Education, Mrs. Lucia Figar, the Counsellor of Economy, Mr. Enrique Ossorio, the Mayor of Getafe as well as by many members of the Board of Trustees and of the Scientific Council of IMDEA Materials Institute. After the inauguration ceremony, Mr. González visited the new laboratories where the Institute scientists explained the different research activities under development.

Figure 3. The President of the Regional Government of Madrid, Mr. Ignacio González, during the official inauguration of the building.

Figure 4. The Director of IMDEA Materials, Prof. LLorca, explains to Mr. González the details of an experiment to optimize processing of polymer matrix composites for aerospace.

The Institute is located in Tecnogetafe, a scientific and technological park created by a joint venture of the Regional Government of Madrid and the Municipality of Getafe which is located 16 Km to the south of Madrid. With an area close to 1 million of square meters, it is one of the largest of its kind in Europe and houses both industrial enterprises as well as research centres, as the research centre for composite materials of EADS (FIDAMC).

Tecnogetafe also includes the Scientific and Technological Park of the Polytechnic University of Madrid, which counts with several research laboratories in energy, aerospace, materials and electrical engineering and Centesil, a facility devoted to the processing of Si wafers for solar energy generation.

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

1.5. Governing Bodies

1.5.1. Members of the Board of Trustees

CHAIRMAN OF THE FOUNDATION

Dr. Pedro Muñoz-Esquer
Independent Consultant

VICE-CHAIRMAN OF THE FOUNDATION

Excma. Sra. Dª. Lucía Figar de Lacalle
Counsellor of Education, Youth and Sports
Madrid Regional Government

PERMANENT TRUSTEES (REGIONAL GOVERNMENT)

Excma. Sra. Dª. Lucía Figar de Lacalle
Counsellor of Education, Youth and Sports
Madrid Regional Government

Ilmo. Sr. D. Jon Juaristi Linacero
General Director for Universities and Research
Madrid Regional Government

Dr. Juan Ángel Botas Echevarría
Deputy General Director for Research
Madrid Regional Government

Mr. José de la Sota Rius
Managing Director
Fundación para el Conocimiento (Madri+d). Madrid

UNIVERSITIES AND PUBLIC RESEARCH INSTITUTIONS

Prof. Juan Manuel Rojo
Professor
Complutense University of Madrid

Prof. Victor Ramón Velasco
Research Professor
Eduardo Torroja Institute for Construction Science (CSIC). Spain

Prof. Manuel Elices
Professor
Polytechnic University of Madrid

Prof. Carlos Balaguer
Professor
Carlos III University of Madrid

SCIENTIFIC TRUSTEES

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

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

Dr. Pedro Muñoz-Esquer
Independent Consultant, Spain

Prof. Trevor William Clyne
Professor
Cambridge University, UK

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

EXPERT TRUSTEES

Mr. Pedro Escudero
Managing Director
Banco Espírito Santo Spain, Spain

COMPANIES TRUSTEES

AIRBUS OPERATIONS S.A.
Dr. José Sánchez Gómez
Head of Composite Materials
Getafe, Madrid, Spain

ACITURRI AERONAUTICA S.L.
Ms. Francisa Rodríguez.
Director of Engineering
Tres Cantos, Madrid, Spain

GRUPO ANTOLIN S.A.
Mr. Fernando Rey
Director of Innovation and Marketing
Burgos, Spain

GAMESA S.A.
Mr. José Antonio Malumbres
General Director of Technology
Sarriguren, Navarra, Spain

INDUSTRIA DE TURBOPROPULSORES S.A.
Dr. José Ignacio Ulizar
Director of Technology
San Fernando de Henares. Madrid, Spain

SECRETARY

Mr. Alejandro Blázquez

1.5.2. Members of the Scientific Council

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

Prof. Brian Cantor
Vice-chancellor
York University, UK

Prof. Trevor W. Clyne
Professor
Cambridge University, UK

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

Prof. Manuel Elices
Professor
Polytechnic University of Madrid, Spain

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

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

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

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

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

Prof. Pedro Muñoz-Esquer
Independent consultant

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

Prof. Gary Savage
Independent consultant

Prof. John R. Willis
Professor
Cambridge University, UK

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

research

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2.1. Research Programmes

The research activities of IMDEA Materials Institute are organised within four research programmes devoted to:

- Nanomaterials and Nanomechanics
- The Next Generation of Composite Materials
- Alloy Design, Processing and Development
- Integrated Computational Materials Engineering

Each research programme combines the expertise of different research groups (processing, characterization and simulation) leading to a multidisciplinary effort to achieve results beyond the state-of-the-art. Moreover, knowledge transfer between different research programmes is promoted by the fact that different research groups are often involved in two or more research programmes.

These programs are focused on the development of advanced materials mainly in the sectors of transport, energy, information technology and manufacturing as well as on the exploration of emerging materials and processes for sustainable development. Driven by the talent of the researchers, they combine cutting-edge fundamental oriented research in topics at the frontiers of knowledge with applied research encompassing the midterm interest of our industrial partners to provide long-term technological leadership.

Figure 5. Research programmes and strategic partners of IMDEA Materials Institute

futurefibres
Tomorrow's innovation

Thomas Swan
Chemical manufacturing since 1926

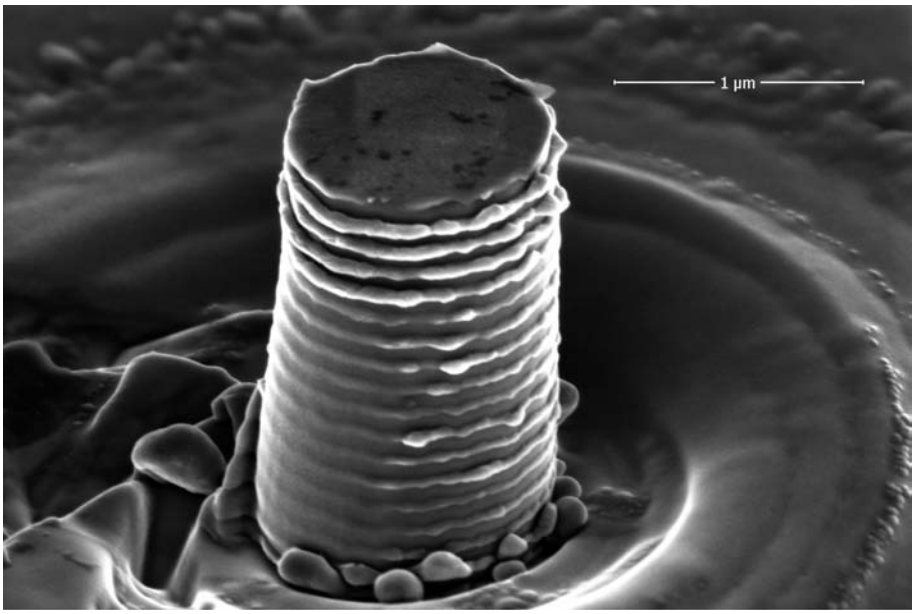
INAEL

Nanomaterials and Nanomechanics

- Graphene, nanotubes, CNT fibres and hybrids. Synthesis, emerging properties and micro/macroscopic applications.
- Nanomaterials for energy generation and storage
- Hierarchical materials
- Sustainable materials (bio-based nanocarriers, nano-fire retardant, novel guest-host nanomaterials, fire retardant polymer nanocomposites, etc.)
- Nanoscale multilayers for extreme environments (high temperature coatings, radiation resistant applications, etc.)
- High temperature nanomechanics
- In situ characterization of materials at the nm and μm scale

Research groups

- Multifunctional Nanocomposites (Dr. J. J. Vilatela)
- Nano-architectures and Materials Design (Dr. R. Guzmán de Villoria)
- High Performance Nanocomposites (Dr. D.-Y. Wang)
- Nanomechanics (Dr. J. M. Molina-Aldareguía)
- Multiscale Materials Modeling (Dr. J. Segurado)
- Mechanics of Materials (Prof. J. LLorca)
- Hybrid polymer nanocomposites (Dr. A. Dasari)



The Next Generation of Composite Materials

- Low-cost techniques for processing high performance composites (out-of-autoclave, hot-forming, in-situ consolidation of thermoplastics)
- Recycling and reparability of structural composites
- New frontiers of structural performance (high temperature, impact, self-healing, smart materials, self-sensing, non-conventional lay-up configuration, etc.)
- Composites with multifunctional capabilities (fire resistance, electrical and thermal conductivity, barrier properties, etc.)
- Micromechanics-based constitutive equations of mechanical behaviour including the effect of ageing and service conditions
- Multiscale modelling strategies for virtual testing and virtual optimization of composite materials and structures

Research groups involved:

- Structural Composites (Dr. C. González)
- Design & Simulation of Composite Structures (Dr. C. Lópes)
- Multifunctional Nanocomposites (Dr. J. J. Vilatela)
- Nano-architectures and Materials Design (Dr. R. Guzmán de Villoria)
- High Performance Nanocomposites (Dr. D.-Y. Wang)
- Nanomechanics (Dr. J. M. Molina-Aldareguía)
- Mechanics of Materials (Prof. J. LLorca)

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Novel Alloy Design, Processing and Development

- Metallic alloys for high temperature structural applications (Ni/Co-based superalloys, TiAl and NiAl intermetallics, etc.)
- Lightweight (Mg, Al, Ti) alloys and their composites
- Physical simulation for developing optimal thermo-mechanical processing routes for metallic materials
- Stabilization of novel metastable metallic phases under ambient conditions
- High throughput and diffusion techniques

Research groups involved:

- Metal Physics (Dr. M. T. Pérez-Prado)
- Solid State Processing (Prof. J. M. Torralba)
- Solidification Processing and Engineering (S. Milenkovic)
- Physical Simulation (Dr. I. Sabirov)
- Multiscale Materials Modeling (Dr. J. Segurado)
- Computational Alloy Design (Dr. Y. Cui)
- High-Temperature Alloys (Dr. C. J. Boehlert)

Integrated Computational Materials Engineering

ABENGOA RESEARCH

- Virtual materials design, including virtual processing and virtual testing
- Multiscale materials modelling (molecular mechanics, MonteCarlo, computational thermodynamics, phase-field, dislocation dynamics, finite element, homogenization, etc.)
- Active and smart materials (electro-active polymers, magneto-rheological elastomers, etc.)

ITP the power of talent

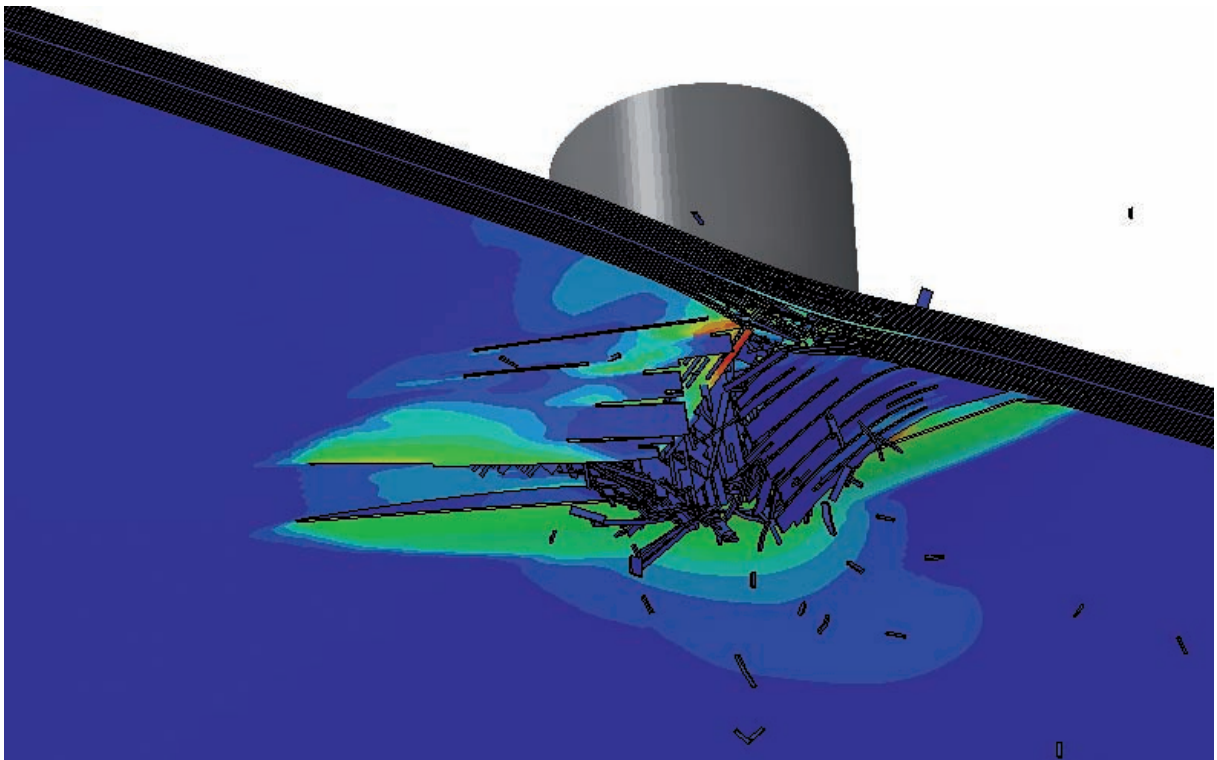
SYNOPSYS®

GLOBALFOUNDRIES®

Research groups involved:

- Mechanics of Materials (Prof. J. LLorca)
- Atomistic Materials Modelling (Dr. I. Martín-Bragado)
- Multiscale Materials Modelling (Dr. J. Segurado)
- Computational Alloy Design (Dr. Y. Cui)
- Theoretical and Applied Mechanics (Prof. P. Ponte-Castañeda)
- Computational Mechanics of Materials (Dr. A. Jérusalem)

eXstream ENGINEERING MSC Software Company



people

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IMDEA Materials Institute is committed to attract talented researchers from all over the world to Madrid to work in an international and interdisciplinary environment. The Institute counts currently with 65 Researchers, including 9 Senior Researchers, 7 Researchers, 3 Visiting Scientists, 14 Postdoctoral Research Associates, and 32 Research Assistants from 15 different nationalities. It should be noted that 50% of the researchers are foreign nationals while 61% of the PhD were granted by foreign universities. This international team with multidisciplinary expertise is contributing to establish IMDEA Materials Institute as an international reference in Materials Science and Engineering.

The researchers are supported by 3 Laboratory Technicians and the Management and Administrative staff, including an international Project Management team.

senior researchers

Prof. Javier LLorca

Director,
Mechanics of Materials

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

Professor of Materials Science, Polytechnic University of Madrid.

Research Interests

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

Prof. Jose Manuel Torralba

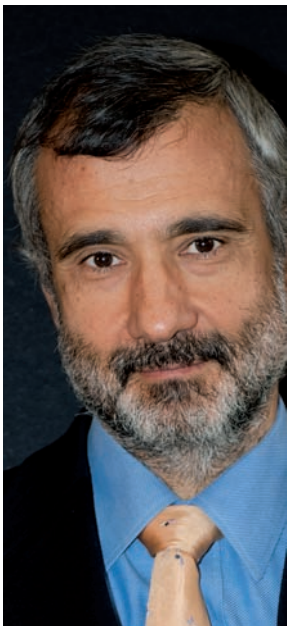
Deputy Director,
Solid State Processing

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

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

Research Interests

Manufacturing of advanced structural materials by powder metallurgy; development of new alloying systems to improve sintering behaviour and structural properties of low-alloy steels, special steels (stainless and high speed steels) with improved corrosion and wear resistance, and metal-matrix composites, including different matrix materials as aluminium, iron or high speed steel; and processing technologies as mechanical alloying, metal injection moulding or spray pyrolysis to manufacture nanoparticles.



Dr. Carlos González
Senior Researcher,
Structural Composites

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

Associate Professor of Materials Science, Polytechnic University of Madrid

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

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

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

Research Interests
Micromechanics and Nanomechanics of multifunctional materials; microstructural and mechanical characterization of thin-films, multiphase materials using nanoindentation and advanced focus-ion beam and electron microscopy analysis, mechanical testing inside the scanning electron microscope.

Dr. María Teresa Pérez-Prado
Senior Researcher,
Metal Physics

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

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

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

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

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

Research Interests
Development of theoretical models for the physical and mechanical properties of heterogeneous material systems, specializing in nonlinear properties, microstructure evolution and applications to metal- and polymer-matrix composites, polycrystalline materials, active materials and geo-materials.

Dr. Ilchat Sabirov

Senior Researcher,
Physical Simulation

Ph.D. in Metallurgy from Montanuniversitaet Leoben. Austria

Research Interests

Deformation processing of metallic materials and its effect on the microstructure and properties; physical simulation of metallurgical processes; development of unique thermo-mechanical processing routes to optimize the multifunctional performance of metallic materials.

Dr. Javier Segurado

Senior Researcher,
Multiscale Materials Modelling

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

Associate Professor of Materials Science, Polytechnic University of Madrid

Research Interests

Multiscale modelling of structural materials; physically-based models to simulate the mechanical behaviour of metals at different length scales: molecular dynamics, discrete dislocation dynamics and single-crystal plasticity; computational homogenization and concurrent multiscale modelling techniques for polycrystalline materials; computational micromechanics strategies to simulate the mechanical behaviour until failure of both particle- and fibre-reinforced composites.

Dr. De-Yi Wang (2012 new incorporation)

Senior Researcher,
High Performance Nanocomposites

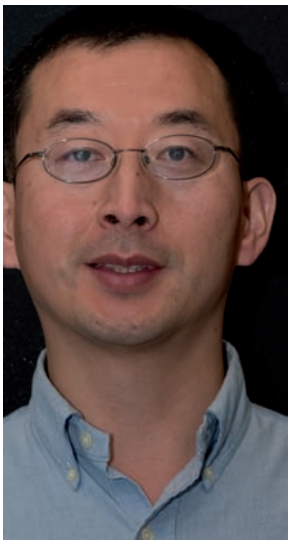
Ph.D. in Polymer Chemistry and Physics from Sichuan University. China

Dr. De-Yi Wang holds a MSc (2004) from Sichuan University, China and got his PhD at the same institution in 2007, conducting part of his doctoral research at the University of Bolton in United Kingdom. His research activities on fire retardant materials and high performance polymeric materials continued at College of Chemistry, Sichuan University, where he was appointed lecturer in 2007. In 2008, he joined Leibniz-Institut für Polymerforschung Dresden e. V. in Germany as a visiting scientist, working on the development of environment-friendly fire retardant materials. He was promoted to Associate Professor in Polymer Composites in Sichuan University in 2009 and obtained an Alexander Humboldt Fellowship to continue his research activities in Dresden. In 2010, Dr. Wang research contributions were recognized with the DuPont Young Professor Award. He joined IMDEA Materials Institute as Senior Researcher in 2012 where he leads the research group of High Performance Polymer Nanocomposites. He is an Academic Consultant on environmentally friendly chemical materials of the United Nations Industrial Development Organization (UNIDO) since 2012. Dr. Wang has published more than 50 academic papers in peer-reviewed international journals and is co-inventor of 16 patents.

Research Interests

Application-oriented fundamental problems and novel technologies in multifunctional nanomaterials, eco-benign fire retardants, high performance environment-friendly polymers and nanocomposites (bio-based and/or petro-based). Synthesis and modification of novel multifunctional nanostructure materials, design and processing of high performance polymers and their nanocomposites, with particular emphasis in structural properties and behaviour under fire.

researchers



Dr. Yuwen Cui

Researcher,
Computational Alloy Design

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

Research Interests

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

Dr. 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. Ignacio Martin-Bragado

Researcher, Atomistic Materials Modelling

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

Research Interests

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

Dr. Srdjan Milenkovic

Researcher,
Solidification Processing
& Engineering

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

Research Interests

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

Dr. Roberto Guzmán de Villoria

Researcher,
Nano-Architectures and
Materials Design

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

Research Interests

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

Dr. Claudio Saul Lopes

Researcher,
Design & Simulation of
Composite Structures

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

Research Interests

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

Dr. Juan José Vilatela

Researcher,
Multifunctional
Nanocomposites

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

Research Interests

Nanocomposite materials, produced by controlled assembly from the nano to the macroscale, where the possibility of hierarchical tailoring provides materials with multifunctional properties (e.g. mechanical, thermal), often superior to those of conventional materials, and makes them suitable for a wide variety of applications; carbon nanotubes, CNx, inorganic nanotubes (e.g. TiO2), cellulose, graphene and silica nanoparticles as well as thermoset, elastomeric and thermoplastic matrices; applications of Raman spectroscopy and synchrotron X-ray diffraction to study the structural evolution of materials under mechanical deformation.

visiting researchers

Dr. Carl J. Boehlert

Visiting Scientist,
High-temperature Alloys

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

Associate Professor. Department of Chemical Engineering and Naturals Science. Michigan State University. USA.

Research Interests

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

Dr. Aravind Dasari

Visiting Scientist,
Multifunctional
Nanocomposites

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

Assistant Professor. Department of Naturlas Science and Enginnering. Nanyang Technological University. Singapore.

Research Interests

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

Prof. Patricia Frontini

Visiting Scientist,
Polymers and Composites

Ph.D. in in Materials Science, Universidad Nacional de Mar de Plata. Argentina

Faculty of Engineering. University of Mar del Plata. Argentina

Research Interests

Elasticity, viscoelasticity, fracture mechanics, plasticity and failure micromechasism of polymers, micro and nanocomposites, natural polymers and structural composites; evaluation of surface and tribological properties and the determination of viscoelastic-viscoplastic constitutive equations through nanoindentation.

postdoctoral research associates

Dr. Michalis Agoras
Postdoctoral Research Associate

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

Research Interests

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

Dr. Somjeet Biswas
Postdoctoral Research Associate

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

Research Interests

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

Dr. Juan Pedro Fernández
Postdoctoral Research Associate

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

Research Interests

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

Dr. Paloma Hidalgo
Postdoctoral Research Associate

Ph.D. in Physical Metallurgy from Complutense University of Madrid. Spain

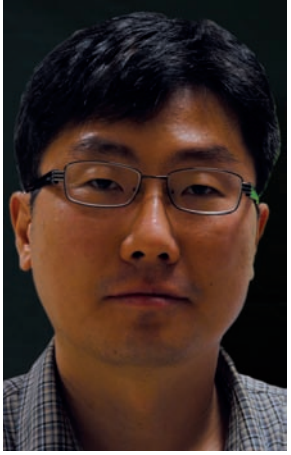
Research Interests

Study of recrystallization and deformation mechanisms of metallic materials and their microstructural characterization by means of optical / electronic microscopy and texture analysis.

Dr. Nianjun Kang
Postdoctoral Research Associate

Ph.D. in Materials Science and Engineering, Beijing University of Chemical Technology, China

Research Interests
Design, synthesis and characterization of environmentally friendly fire retardant materials, multifunctional nanomaterials and polymer nanocomposites.



Dr. Dong-Wook Lee
Postdoctoral Research Associate

Ph.D. in Mechanical Engineering from Texas Tech University, USA

Research Interests
Phase field modeling of solid-state phase transformation, mesoscale modeling of dislocation and fracture.

Dr. Miguel Monclús
Postdoctoral Research Associate

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

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

Dr. Raghu Raja
Postdoctoral Research Associate

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

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

Dr. Jerome Rajakesari
Postdoctoral Research Associate

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

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

Dr. Srinivasa Rao Bonta
Postdoctoral Research Associate

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

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

Dr. Rocio Seltzer

Postdoctoral Research Associate

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

Research Interests

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

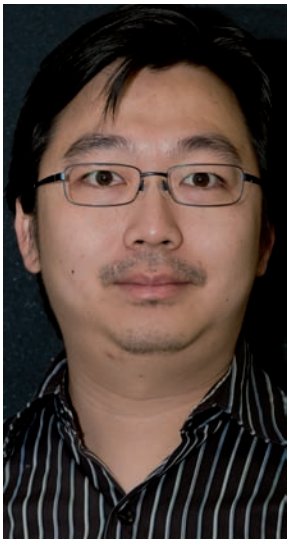
Dr. Federico Sket

Postdoctoral Research Associate

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

Research Interests

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



Dr. Denny Tjahjanto

Postdoctoral Research Associate

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

Research Interests

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

Dr. Guillermo Vigueras

Postdoctoral Research Associate

Ph.D. in Computer Science from University of Valencia, Spain.

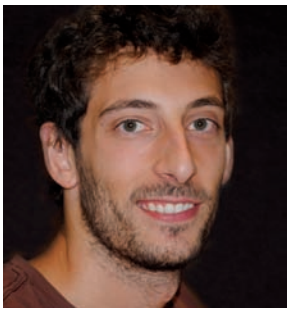
Research Interests

High Performance Computing (HPC) aspects of the modelling and simulation of materials at different scales, from the atomistic to the macroscopic scale.

research assistants

Laura Agudo

M.Eng.: Rey Juan Carlos University. Spain
Research: Multiscale Materials Modelling



Alexandros Charalambides

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

Yi Chen

M.Eng.: Northwestern Polytechnical University. China
Research: Thermo-Kinetic Study of Near Beta Ti Alloys

María Irene de Diego

M.Eng.: Carlos III University. Spain
Research: Advanced High Strength Steels

Ignacio Dopico

M.Eng.: Autonomous University of Madrid, Spain
Research: Multiscale Materials Modelling

Nathamar Dudamell

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

Hossein Ehteshami

M.Eng.: Bahonar University of Kerman. Iran.
Research: Multiscale Materials Modeling

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

Silvia Hernández

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

Mohammad Ali Jabbari

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

Saeid Lotfian

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

Francisca Martínez

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

Bartolomé Mas

MEng: Polytechnic University of Madrid. Spain
Research: Multifunctional Composites based on CNT Fibres

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

Raul Muñoz

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

Ehsan Naderi Kalali

M.Eng.: Pune University. India
Research: High-performance Polymer Nanocomposites

Fernando Naya

M.Eng.: Polytechnic University of Madrid. Spain
Research: Multiscale Simulation of Composites

Nithin Palavalli

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

Mehdi Rahimian

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

Pablo Romero

M.Eng.: Polytechnic University of Madrid. Spain
Research: Nano-Architectures and Materials Design

Marcos Rodriguez

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

Raúl Sánchez

M.Eng.: University of Cantabria. Spain
Research: Nanoindentation of Light Alloys

José Luis Selles

M.Eng.: Complutense Univesrsity of Madrid. Spain
Research: Multiscale Materials Modelling

Rafael Soler

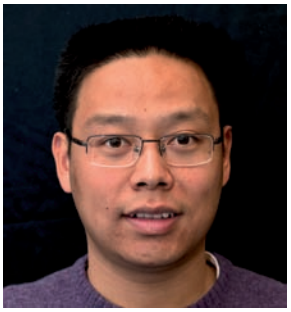
M.Eng.: Cranfield University. UK
Research: Nanomechanics

Arcadio Varona

M.Eng.: Rey Juan Carlos University. Spain
Research: Advanced NiAl-based Eutectic Alloys

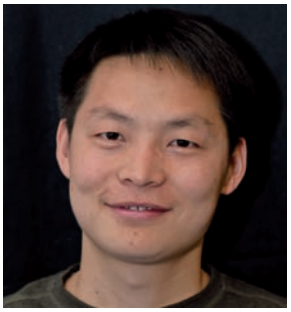
Joaquim Vilà

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



Guanglong Xu

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



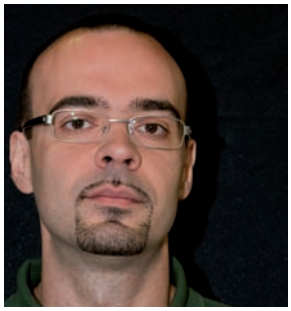
Hangbo Yue

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

Xiaomin Zhao

M.Eng.: Shanghai Jiao Tong University. China
Research: Polymer Nanocomposites

laboratory technicians



José Luis Jiménez

V.T.: Specialist Technician. Spain

Vanesa Martínez

M.Eng.: University of Valencia. Spain

Juan Carlos Rubalcaba

B.Eng.: Alcalá de Henares University. Spain

management and administration

Dr. Covadonga Rosado
Manager

Miguel Ángel Rodiel
Technology Manager

Vanessa Fernández
Personnel Manager

Eduardo Ciudad-Real
Accountant Responsible

Borja Casilda
Accountant Assistant

Elena Bueno
Secretary

scientific infrastructures

annual report 2012

4.1. Processing

- **Carbon Nanotube Fibre Spinning Reactor** (built in-house, IMDEA Materials Institute) to produce continuous macroscopic fibres made out of CNTs directly spun from the gas-phase during chemical vapour deposition. It can produce kilometres of fibre per day, at rates between 10 – 50 m/min.

- **Horizontal Chemical Vapor Deposition** (CVD) Reactor (built in-house, IMDEA Materials Institute) to carry out nano-structure synthesis, such as vertically aligned carbon nanotubes, nanorods or graphene. The system has been automatized to control all the synthesis parameters (Tmax=1200 °C).

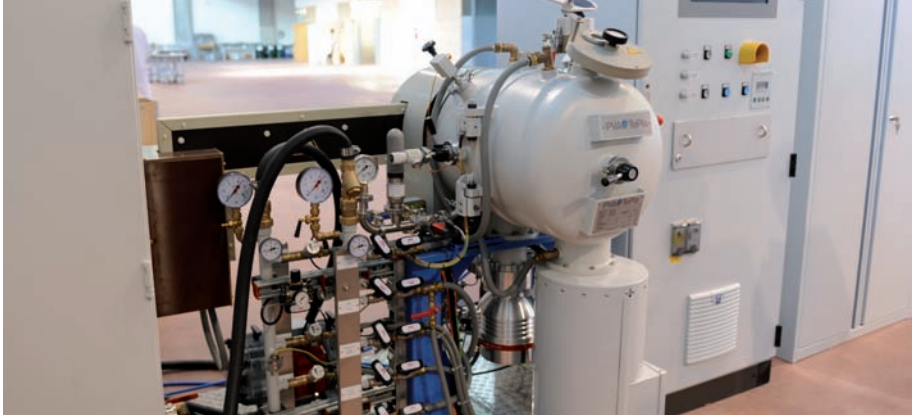
- **Vacuum Induction Melting and Casting System** (VSG 002 DS, PVA TePla) to melt a wide range of metals, alloys or special materials under high vacuum, fine vacuum or different gas atmospheres with subsequent casting into moulds or forms. In addition, it is equipped with a directional solidification device, which enables growth of single crystals and aligned columnar structures.

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

- **Pultrusion Line** (design in-house, IMDEA Materials Institute) 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.

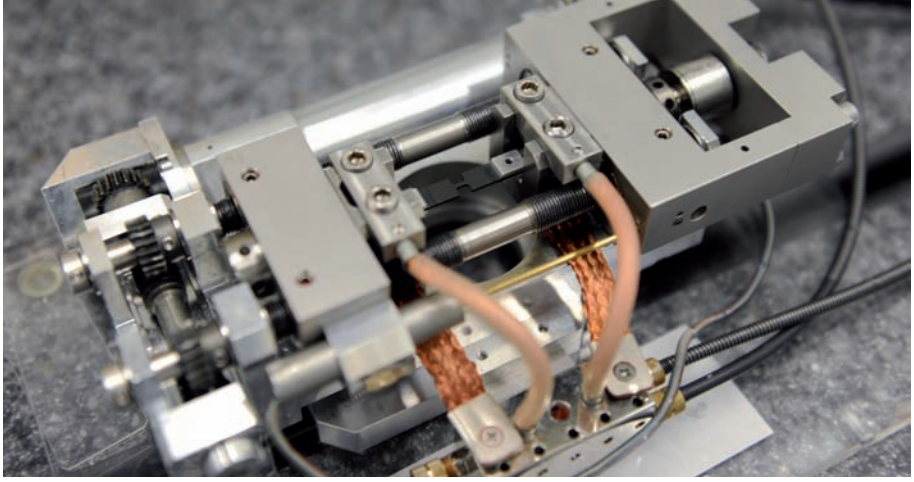
4.2. Microstructural Characterization

- **Ultrasound non-destructive Inspection System, C-Scan** (Triton 1500, Tecnitest) to detect and evaluate defects by non-destructive ultrasounds technique. The system finds and determines the size and position of the typical defects in composite materials (voids, delaminations, cracks, etc).

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

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

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



- **X-ray Computer-assisted 3D Nanotomography Scanner** (Nanotom, Phoenix) for three-dimensional visualization and quantitative analysis of microstructural features in a wide variety of materials ranging from metal powders and minerals to polymers and biomaterials. The scanner combines a 160 KV X-ray source to study highly absorbing materials together with a nanofocus tube to provide high resolution (0.2-0.3 µm detail detectability).

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

4.3. Mechanical Characterization

- **High Temperature Nanoindentation System** (Nanotest Vantage, Micro Materials) to perform instrumented nanoindentation at temperatures up to 750°C, and also in inert environments. The instrument uses both tip and sample heating, ensuring stability for long duration testing, including creep tests. This is the first dedicated high temperature nanoindentation instrument in Spain.

- **Mechanical Stage for in-situ Testing in X-ray Tomography** (µTM, built in-house, IMDEA Materials Institute) to carry out in-situ mechanical tests under X-ray radiation in computer assisted tomography systems. The stage, designed and developed in-house, can be used both at synchrotron radiation facilities and inside laboratory tomography systems, for the investigation of the damage initiation and propagation in a wide variety of materials.

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

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

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

- **Micromechanical Testing Stages** (Kammrath and Weiss) to observe the specimen surface upon loading under light, scanning electron, focused ion-beam, scanning ultrasonic, or atomic force microscopy. Two stages for tension/compression and fibre tensile testing are available, with maximum loads of 10 kN and 1 N, respectively. A heating unit allows to carry out tests up to 700ºC.

- **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.

4.4. Thermal Characterization

- **Thermal Conductivity Analyser** (TPS 2500 S Hot Disk) to measure thermal conductivity of samples based on a transient method technique. The equipment can be used to measure a wide variety of samples, from insulators to metals, as well as to determine thermal diffusivity in anisotropic materials.

- **Dual Cone Calorimeter** (Fire Testing Technology) to study the forced combustion behaviour of polymers simulating real fire conditions; fire relevant properties including time-to-ignition, critical ignition flux heat release rates (HRRs), peak of HRR, mass loss rates (MLRs), smoke production, CO2 and CO yields, effective heat of combustion, and specific extinction areas are directly measured according to ASTM/ISO standards.

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

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

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

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

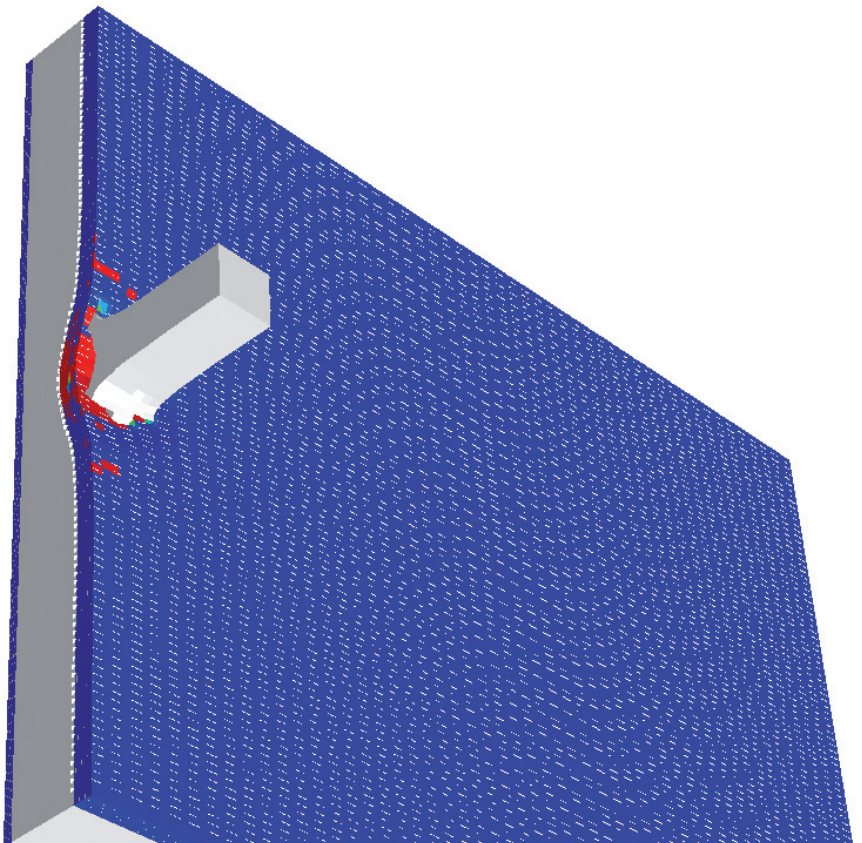
- **High Temperature Furnace** (Nabertherm, RHTH 120/600/16) to carry out heat treatments of up to temperatures of 1600ºC in vacuum or in an inert atmosphere.

4.5. Simulation

- **High Performance Computing Cluster** (236 cores, AMD Opteron)

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

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



research projects

annual report

2012

IMDEA Materials Institute currently participates in 39 research projects, 12 of which began in 2012. The project funding coming from industrial contracts and European projects increased by 51% and 60%, respectively, with respect to the previous year. The project portfolio is divided into three main groups: 18 projects were obtained in international competitive calls, out of which 13 are funded by the European Union, 4 by the Chinese Scholarship Council and 1 is jointly supported by the National Science Foundation of the US and the Spanish Ministry of Economy and Innovation (MINECO) within the Materials World Network Programme. 6 projects are supported by research programs sponsored by MINECO and the Regional Government of Madrid, while 15 projects are directly funded through industrial contracts. Several of these industrial contracts are supported by the Spanish Centre for Technological and Industrial Development (CDTI).

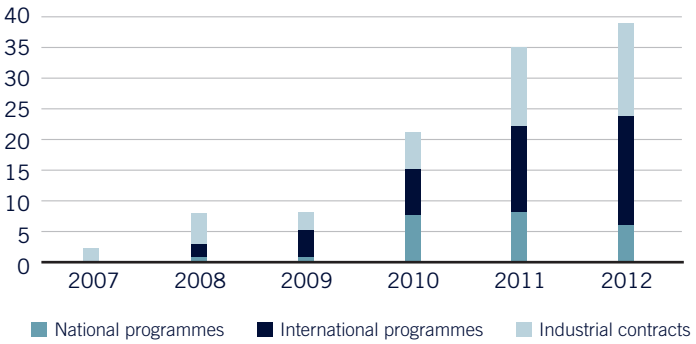


Figure 6. Active research projects by funding source

A brief description of several projects started in 2012 is provided below

SEVENTH FRAMEWORK PROGRAMME

EXOMET

"Physical processing of molten light alloys under the influence of external fields"

Funding: **NMP, European Union-7th Framework Programme**
Partners: Consortium of 26 European partners coordinated by the European Space Agency (ESA)
Duration: **2012-2016**
Principal Investigators: **Dr. J. M. Molina-Aldareguía and Dr. M. T. Perez-Prado**

The core concept of the ExoMet project involves developing new liquid metal processing techniques coupled with external fields. These techniques will revolutionise microstructure control in metallic alloys and their composites, and allow for properties not reachable by conventional processing routes and compositions. The metals of greatest interest in this proposal are Mg and Al alloys, although the proposed methods will also be of

high value to other alloy systems in the future (e.g. titanium, copper, steel, cobalt, nickel, zinc, intermetallics, high entropy alloys, bulk metallic glasses etc). The use of external fields (electromagnetic, ultrasonic and intensive mechanical shearing) to disperse novel grain refiners and nanoparticle reinforcers into melts and the subsequent solidification of light alloy nanocomposites are key topics to be addressed in ExoMet. IMDEA Materials contribution focuses on the study of the microstructure-processing-deformation relationship including the high temperature behavior, both at the macroscopic and microscopic levels.

MUFIN

"Multifunctional fibre nanocomposites"

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**
Duration: **2012-2016**
Principal Investigator: **Dr. J. J. Vilatela**

SEVENTH FRAMEWORK PROGRAMME

MARIE CURIE ACTIONS

The subject of this project is the production and study of new composites with multifunctional properties, including mechanical properties in the high-performance range and electrical and thermal conductivities superior to those of carbon fibre. The composites will be similar to standard fibre-reinforced polymer composites, but they will be reinforced with a new type of high-performance fibre entirely made up of carbon nanotubes and which has a unique combination of mechanical, electrical and thermal properties. The aim is to develop the science to integrate the fibres and matrix in a way that the composite structure is tailored throughout different scales. Thus, the outstanding properties of carbon nanotubes are simultaneously and efficiently exploited on a macroscopic scale composite that can be the basis for multiple applications (structural composites, damage sensing, heat management, etc).

SIMSCREEN

"Simulation for screening properties of materials"

Funding: **Airbus Operations S.A.S. (France)**
Duration: **2012-2014**
Principal Investigator: **Dr. C. González**

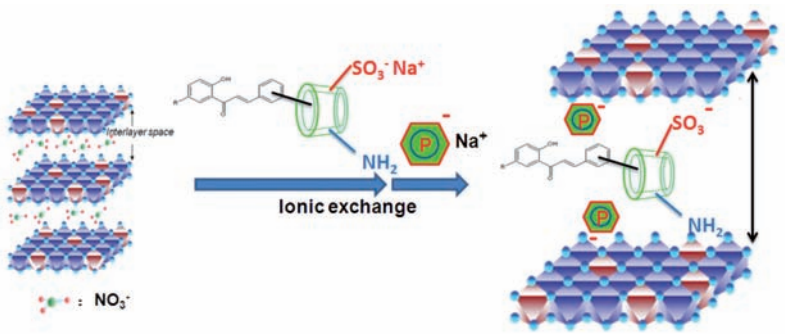
This two years industrial contract between Airbus Operations France and IMDEA Materials Institute aims at reducing the number of tests necessary to fully characterize by experimental campaigns standard unidirectional carbon composite material. To this end, a coupled experimental-computational micromechanical framework will be used. The purpose is to extend the testing pyramid at the base by including additional tests at the constituent level (fibre, matrix, interface) and use micromechanical models to compute ply properties which can be used in the design and certification of composite materials and structures.

ECOFIRENANO

"New generation of eco-benign multifunctional layered double hydroxide (LDH)-based fire retardant and nanocomposites"

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**
Duration: **2012-2016**
Principal Investigator: **Dr. D.-Y. Wang**

Fire retardants can significantly improve the fire safety of the materials leading to enhance security and reduction of risks in the case of fire. The development of novel eco-benign, high performance fire retardants and materials is atractive not only from industrial but also from environmental and socio-econpmical standpoints. This project presents an interdisciplinary and innovative approach to design a new generation of eco-benign multifunctional Layered Double Hydroxides(LDH)-based fire retardant nanocomposites in which LDH will be modified by bio-based multifunctional intumescent fire retardants. A new generation of environment-friendly fire retardant materials with enhanced smoke suppression and multifunctional properties is expected to be developed within the project.



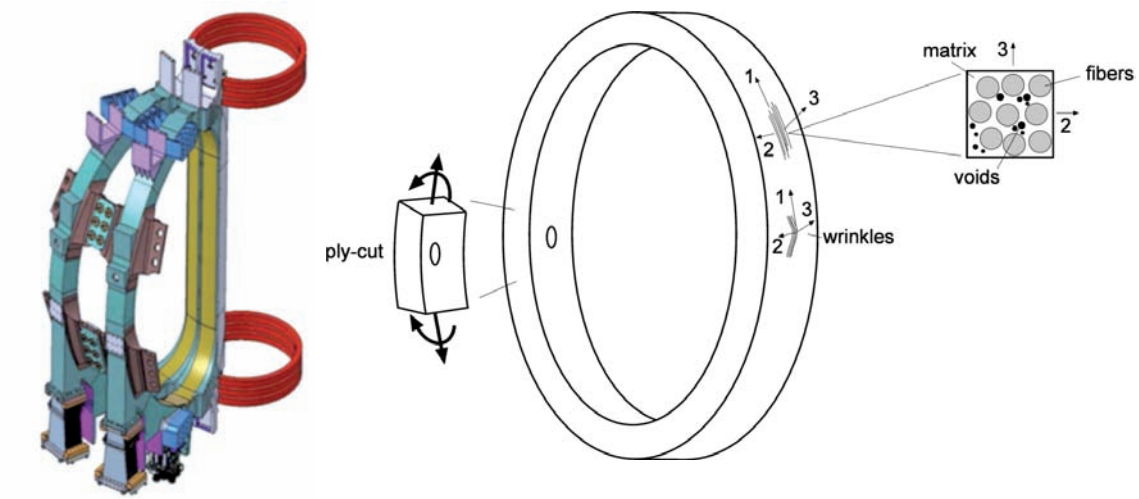
ITER PCR

"Mechanical analysis ITER Pre-Compression Rings"

Funding: EADS CASA Espacio
Duration: **2012-2014**
Principal Investigator: **Dr. C. González**

ITER (acronym of *International Thermonuclear Experimental Reactor*) is an international nuclear fusion research and engineering project, which is currently building the world's largest experimental tokamak nuclear fusion reactor at the Cadarache facility in the south of France. The ITER project aims to make the long-awaited transition from experimental studies of plasma physics to full-scale electricity-producing fusion power plants. The project is funded and run by seven member entities including the European Union, India, Japan, China, Russia, South Korea and the United States. The European Union, as host party for the ITER complex, is contributing 45% of the cost, with the other six parties contributing 9% each.

The pre-compression rings of the ITER magnet system will tightly hold the Toroidal Field (TF) coils on top and bottom with a radial force of 7,000 tons per coil. The most suitable material to withstand such high loads and avoid circulation of currents during machine operation is glass-fiber/epoxy composite. The ITER pre-compression rings are possibly the most massive composite structures ever attempted and will be manufactured by EADS CASA Espacio under contract from ITER. IMDEA Materials Institute is another partner in this contract and it is responsible of mechanical simulation of the mechanical behavior of the pre-compression rings at ambient and operation temperature (4K) by means of advanced multiscale simulation tools.



SEVENTH FRAMEWORK PROGRAMME

MARIE CURIE ACTIONS

NECTAR

"New generation of NiAl-based eutectic composites with tuneable properties"

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**
Duration: **2012-2016**
Principal Investigator: **Dr. S. Milenkovic**

The major objective of the project is to design and develop a new generation of multiphase intermetallic alloys based on NiAl. In contrast to contemporary concepts of alloy design, a novel high-throughput method for systematic microstructure investigation and control will be presented. The greatest challenge will be, however, to obtain a single alloy with high strength and fracture toughness, good ductility and formability, as well as sufficient thermal stability and oxidation resistance.

ABENGOA RESEARCH

VMD

"Virtual materials design"

Funding: **Abengoa Research S.L.**
Duration: **2012-2016**
Principal Investigator: **Prof. J. LLorca**

Abengoa is an international company with headquarters in Spain that applies innovative technology solutions for sustainability in the energy and environment sectors, generating energy from the sun, producing biofuels, desalinating sea water and recycling industrial waste. Abengoa growth model is based on technological leadership.

As part of its long-term research and development strategy, Abengoa Research, in collaboration with universities and research centres, has launched and funded the Virtual Materials Design project. The project is aimed at the development of a simulation platform to perform virtual design, virtual processing and virtual testing of engineering materials to reduce the time necessary to develop and introduce new materials in the market. IMDEA Materials Institute is providing to the project its expertise in modelling of materials (atomistic, computational thermodynamics, phase-field, Monte Carlo, multiscale plasticity) to develop simulation tools at the nano, micro and meso-scale, with the main goal of obtaining a general multi-scale approach to integrated computational materials engineering.

SUPRA NiAl-LOYS

"Computational and experimental design and development of advanced NiAl-based in situ composites with tunable properties"

Funding: **Spanish Ministry of Economy and Competitiveness (Fundamental Research Programme)**
Duration: **2012-2015**
Principal Investigator: **Dr. S. Milenkovic**

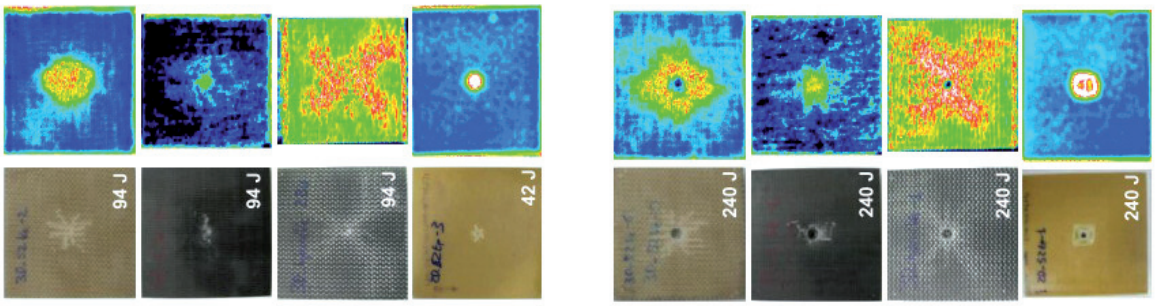
The major objective of the project is to understand, model, design and develop the new class of NiAl-based in situ composites with tunable properties for high temperature services. A novel synergetic approach combining state-of-the-art computational thermodynamics with alloy design, processing and characterization, will be presented. On the one hand, advanced computational thermodynamics will be used to create and optimize thermodynamics databases, which will be subsequently used for constitutional and phase equilibrium calculations. In parallel, diffusion and phase field models will be developed to model the eutectic microstructures resulting from the solidification processing. On the other hand, a combination of sophisticated alloy design and processing will be used to understand the solidification behaviour and control the microstructure. Based on this knowledge the microstructure-property relationship will be established and alloys with superior properties will be tailored.

Pre-HITMAAS

"High temperature material/solution selection"

Funding: **Eurocopter España S.A.**
Duration: **2012-2013**
Principal Investigator: **Dr. R. Guzmán de Villoria**

The goal of this research collaboration is to identify and select new material concepts for possible use and incorporation into the future rear fuselages which operate at high temperature.



BLADE IMPACT

"Shielding design for engine blade release and impact on fuselage"

Funding: **Airbus Operations S.L.**
Duration: **2012-2013**
Principal Investigators: **Dr. C. S. Lopes and Dr. C. González**

This is an industrial contract between AIRBUS Operations and the IMDEA Materials Institute in the framework of the development of the new aircraft family A30X. The project aims at selecting and designing innovative composite shields against the high energy impact of an open-rotor blade on the aircraft fuselage. New materials or combinations thereof, and advanced structural concepts are being evaluated by means of testing and computational mechanical analyses taking into account damage and erosion of materials due to the impact.

ScreenPTK

"Screening of phase transformation kinetics of Ti alloys by high throughput diffusion and mesoscale modeling"

Funding: **Chinese Scholarship Council (China)**
Duration: **2012-2014**
Principal Investigators: **Dr. Y. Cui and Dr. J. Segurado**

Ti and its alloys, widely used in aerospace, chemical and medical industries, exhibit complex microstructures resulting from multiple alloying elements and complex thermo-mechanical processes. The microstructure of Ti alloys is further complicated by the formation of metastable phases like ω (hexagonal structure) and β', leading to alloys whose microstructure is highly sensitive to constituent levels and processing routes. Near β-Ti alloys have been intensively studied in the past using the conventional methods, i.e. one-alloy-at-a-time and one-processing(set)-per-alloy. The ScreenPTK project, with a focus on near β-Ti alloys, aims to develop a high throughput diffusion multiple technique for screening of phase transformation kinetics in Ti alloys, which will be used for quantitative mesoscale modelling of the microstructure.

HIFIRE

"High performance environmentally friendly fire retardant epoxy nanocomposites"

Funding: **Chinese Scholarship Council (China)**
Duration: **2012-2016**
Principal Investigators: **Dr. D.-Y. Wang and Prof. J. LLorca**

Epoxy resin plays a very important role in the development of polymer matrix materials because of their overall superior insulating and mechanical properties. New epoxy-based polymers with enhanced multifunctional properties (e.g. flame retardancy, thermal stability and reduced cost) are required for applications in construction, transportation, aerospace and electric and electronic devices. This project aims at developing high performance fire retardant, halogen-free epoxy nanocomposites by means of molecular design and advanced chemical synthesis. The new nanomaterials will be optimised in terms of nanofiller nature (shape, size and type), loading and dispersion within the epoxy matrix.

Other research projects currently running at IMDEA Materials Institute are:

TRAINER "Smart and self healing technology of materials"

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

MASTIC ("Multi atomistic Monte Carlo simulation of technologically important crystals")

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

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

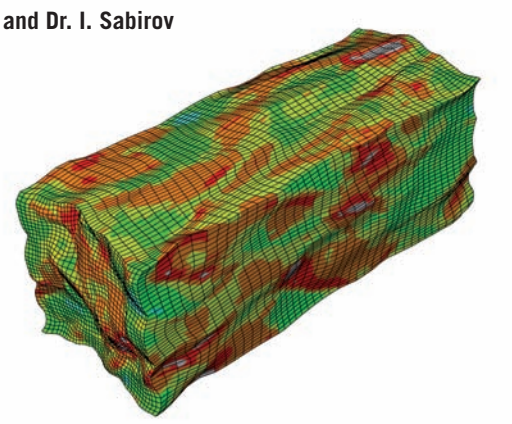
Funding: **NMP, European Union-7th Framework Programme**
Partners: Centre National de la Recherche Scientifique, University of Oviedo, Universidad Politecnica de Madrid, Ecole des Mines de Paris-ARMINES, Czech Technical University in Prague, Universita degli Studi di Cagliari, University of Tartu, Uppsala University, IMDEA Materials Institute, Los Alamos National Laboratory
Duration: **2011-2014**
Principal Investigator: **Prof. J. LLorca**

NewQP ("New advanced high strength steels by the quenching and partitioning process")

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

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

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



SEMICURED ("Semi-cured products manufacturing")

Funding: **Airbus Operations S.L.**
Duration: **2011-2013**
Principal Investigators: **Dr. C. González**

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

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

ASKME ("Atomistic silicon kinetic Monte Carlo modelling for microelectronics")

Funding: **Synopsys Inc. (USA)**
Duration: **2011-2013**
Principal Investigator: **Dr. I. Martin-Bragado**

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

Funding: **Chinese Scholarship Council (China)**
Duration: **2011-2014**
Principal Investigators: **Dr. Y. Cui and Prof. J. LLorca**

SIMET ("Numerical simulations for metallic fragments impact on composites solutions"

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

MASID ("Modelling of advanced semiconductor integrated devices")

Funding: **Global Foundries Singapore Pte Ltd. (Singapore)**
Duration: **2011-2014**
Principal Investigator: **Dr. I. Martin-Bragado**

CAREFIB ("Development of carbon nanotube-based epoxy resins for high performance fibre cables")

Funding: **Future Fibres Rigging Systems S.L. and Centre for Industrial Technological Development (CDTI)**
Duration: **2011-2012**
Principal Investigator: **Dr. J. J. Vilatela**

VIRTEC ("Virtual testing of low-velocity impact on carbon fibre composites")

Funding: **Airbus Operations S. L.**
Duration: **2011-2012**
Principal Investigator: **Dr. C. S. Lopes**

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

Funding: **Chinese Scholarship Council (China)**
Duration: **2011-2014**
Principal Investigators: **Dr. J. J. Vilatela and Prof. J. LLorca**

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: **2010-2013**
Principal Investigator: **Dr. C. González**

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

Funding: **Airbus Operations**
Duration: **2010-2013**
Principal Investigator: **Dr. C. González**

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

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

CAJAL BLUE BRAIN

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

VANCAST ("Next generation nozzle guide vanes")

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

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

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

ELSITEG "Electrospinning of silk fibroin solutions for tissue engineering"

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

HOTNANO ("High temperature nanoindentation")

Funding: **Altare S. L.**
Duration: **2010-2013**
Principal Investigator: **Dr. J. M. Molina-Aldareguía**

ESTRUMAT ("Advanced structural materials")

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

SINTONIA ("Innovative material synergies & composite processing strategies")

Funding: **Centre for Industrial Technological Development (CENIT Programme), Spanish Ministry of Economy and Competitiveness**
Partners: National consortium led by Boeing Research, IMDEA Materials Institute collaborates with Aernnova Engineering Solutions Ibérica and Aries Complex Aeronáutica
Duration: **2010-2013**
Principal Investigator: **Dr. J. Segurado**

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

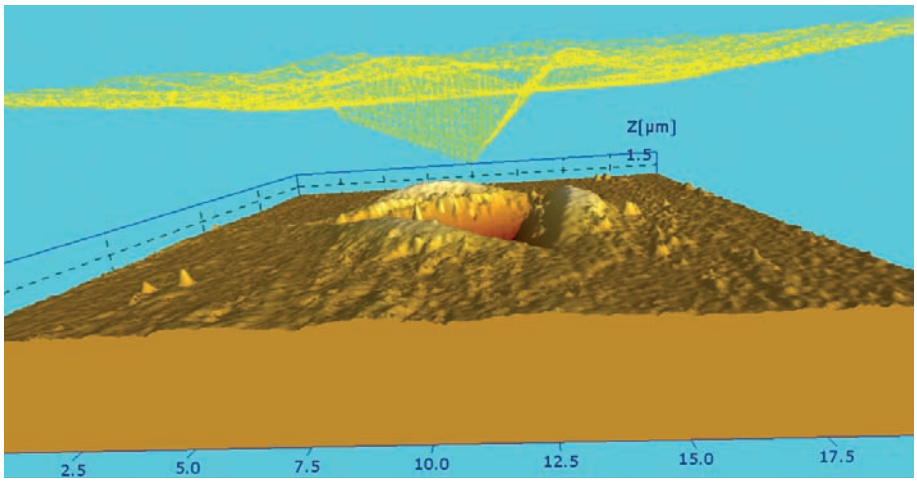
Funding: **Spanish Ministry of Economy and Competitiveness (Fundamental Research Programme)**
Partners: IMDEA Materials Institute and Polytechnic University of Madrid
Duration: **2010-2012**
Principal Investigator: **Dr. J. M. Molina-Aldareguía**

3D-CHARMAT ("3-Dimensional characterisation of materials")

Funding: **Spanish Ministry of Economy and Competitiveness (Integrated Actions Programme)**
Partners: IMDEA Materials Institute and Vienna University of Technology
Duration: **2010-2012**
Principal Investigator: **Dr. J. M. Molina-Aldareguía**

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: **2008-2013**
Principal Investigator: **Prof. J. LLorca**



dissemination of results

annual report 2012

6.1. Publications

1. A. Jérusalem, M. Dao. *Continuum modeling of neuronal cell under blast loading*. **Acta Biomaterialia, 8**, 3360-3371, 2012.

2. Y. Gao, N. Zhou, F. Yang, Y. Cui, L. Kovarik, N. Hatcher, R. Noebe, M. J. Mills, Y. Wang. *P-phase precipitation and its effect on martensitic transformation in (Ni,Pt)Ti shape memory alloys*. **Acta Materialia, 60**, 1514-1527, 2012.

3. M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca. *Determination of the mechanical properties of amorphous materials through instrumented nanoindentation*. **Acta Materialia, 60**, 3953-3964, 2012.

4. J. Frontán Vicente, Y. Zhang, M. Dao, J. Lu, F. Gálvez, A. Jérusalem. *Ballistic performance of nanocrystalline and nanotwinned ultrafine crystal steel*. **Acta Materialia, 60**, 1353-1367, 2012.

5. C. Boehlert, Z. Chen, I. Gutiérrez-Urrutia, J. LLorca, M. T. Pérez-Prado. *In situ analysis of the tensile and tensile-creep deformation mechanisms in rolled AZ31*. **Acta Materialia, 60**, 1889-1904, 2012.

6. R. Soler, J. M. Molina-Aldareguía, J. Segurado, J. LLorca. *Effect of misorientation on the compression of highly anisotropic single-crystal micropillars*. **Advanced Engineering Materials, 14**, 1004-1008, 2012.

7. V. Moroz, J. Huang, G. Letay, I. Martin-Bragado. *Modeling and optimization of solar cells*. **AIP Conference Proceedings**, 201-205, 2012.

8. N. Zographos, C. Zechner, P. Castrillo, I. Martin-Bragado. *Process modeling of chemical and stress effects in SiGe*. **AIP Conference Proceedings, 1496**, 212-216, 2012.

9. Y. Chen, S. Milenkovic, A. Walter Hassel. *Thermal stability of {1 1 0} facet terminated gold nanobelts*. **Applied Surface Science, 258**, 6224–6231, 2012.

10. J. J. Vilatela, R. Khare, A. H. Windle. *The hierarchical structure and properties of multifunctional carbon nanotube fibre composites*. **Carbon, 50**, 1227-1234, 2012.

11. F. Cervantes-Sodi, J. J. Vilatela, J. A. Jiménez-Rodríguez, L. G. Reyes-Gutiérrez, S. Rosas-Meléndez, A. Íñiguez-Rábago, M. Ballesteros-Villarreal, E. Palacios, G. Reiband, M. Terrones. *Carbon nanotube bundles self-assembled in double helix microstructures*. **Carbon, 50**, 3688-3693, 2012.

12. J. J. Vilatela, D. Eder. *Nanocarbon Composites and Hybrids in Sustainability: A Review*. **ChemSusChem, 5**, 456-478, 2012.

13. L. P. Canal, C. González, J. M. Molina-Aldareguía, J. Segurado, J. LLorca. *Application of digital image correlation at the microscale in fiber-reinforced composites*. **Composites Part A, 43**, 1630-1638, 2012.

14. R. Seltzer, Y. Mai and P. M. Frontini. *Creep behaviour of injection moulded polyamide 6/organoclay nanocomposites by nanoindentation and cantilever-bending*. **Composites Part B: Engineering, 43**, 83-89, 2012.

15. F. Sket, R. Seltzer, J. M. Molina-Aldareguía, C. Gonzalez, J. LLorca. *Determination of damage micromechanisms and fracture resistance of glass fiber/epoxy cross-ply laminate by means of X-ray computed microtomography*. **Composites Science and Technology, 72**, 350-359, 2012.

16. L. P. Canal, C. González, J. Segurado, J. LLorca. *Intraply fracture of fiber-reinforced composites: microscopic mechanisms and modeling*. **Composites Science and Technology, 72**, 1223–1232, 2012.

17. N. Lachman, E. Wiesel, R. Guzmán de Villoria, B. L. Wardle, H. D. Wagner. *Interfacial load transfer in carbon nanotube/ceramic microfiber hybrid polymer composites*. **Composites Science and Technology, 72**, 1416-1422, 2012.

publications

18. M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca. *A methodology to measure the interface shear strength by means of the fiber push-in test*. **Composites Science and Technology, 72**, 1924-1932, 2012.

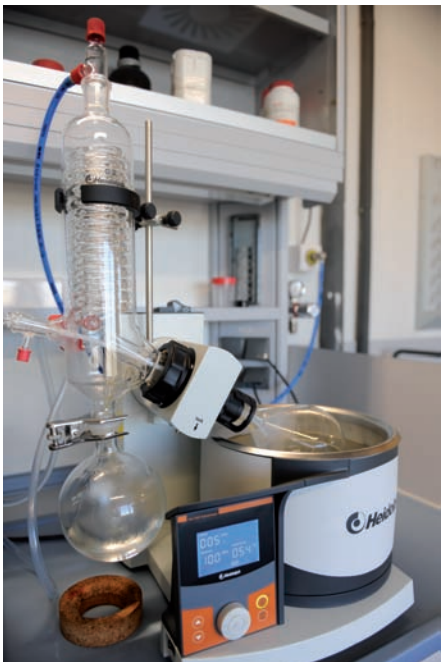
19. M. H. Siboni, P. Ponte Castañeda. *A magnetically anisotropic, ellipsoidal inclusion subjected to a non-aligned magnetic field in an elastic medium*. **Comptes Rendus Mécanique, 340**, 205–218, 2012.

20. A. Ridruejo, C. González, J. LLorca. *Failure locus of polypropylene nonwoven fabrics under in-plane biaxial loading*. **Comptes Rendus Mécanique, 340**, 307–319, 2012.

21. B. Tang, Y.-W. Cui, H. Chang, H. Kou, J. Li, L. Zhou. *A phase-field approach to athermal beta-to-omega transformation*. **Computational Materials Science, 53**, 187-193, 2012.

22. B. Tang, Y.-W. Cui, H. Kou, H. Chang, J. Li, L. Zhou. *Phase field modeling of isothermal $\beta \rightarrow \omega$ phase transformation in the Zr–Nb alloys*. **Computational Materials Science, 61**, 76-82, 2012.

23. H.-B. Yue, Y.-D. Cui, P. S. Shuttleworth, J. H. Clark. *Preparation and characterisation of bioplastics made from cottonseed protein*. **Green Chemistry, 14**, 2009–2016, 2012.



24. A. Ridruejo, C. González, J. LLorca. *Damage localization and failure locus under biaxial loading in glass-fiber nonwoven felts*. **International Journal for Multiscale Computational Engineering, 10**, 425-440, 2012.

25. G. Christou, L. R. Young, R. Goel, A. Vechart, A. Jérusalem. *Shock attenuation of PMMA sandwich panels filled with soda-lime glass beads: a fluid-solid interaction continuum model simulation*. **International Journal of Impact Engineering, 47**, 48-59, 2012.

26. G.-L. Xu, Y.-W. Cui, H. J. Fei, L. G. Zhang, L. B. Liu, Z. P. Jin. *Phase equilibria in the Gd-Ni binary and Mg-Ni-Gd ternary systems*. **International Journal of Materials Research, 103**, 1179-1187, 2012.

27. P. Ponte Castañeda, M. N. Siboni. *A finite-strain constitutive theory for electro-active polymer composites via homogenization*. **International Journal of Non-Linear Mechanics, 47**, 293-306, 2012.

28. J. Segurado, R. A. Lebensohn, J. LLorca, C. Tomé. *Multiscale modeling of plasticity based on embedding the viscoplastic self-consistent formulation in implicit finite elements*. **International Journal of Plasticity, 28**, 124-140, 2012.

29. R. Soler. J. M. Molina-Aldareguia, J. Segurado, J. LLorca, R. I. Merino, V. M. Orera. *Micropillar compression of LiF [111] single crystals: Effect of size, ion irradiation and misorientation*. **International Journal of Plasticity, 36**, 50–63, 2012.

30. E. Galipeau, P. Ponte Castañeda. *The effect of particle shape and distribution on the macroscopic behavior of magnetoelastic composites*. **International Journal of Solids and Structures, 49**, 1-17, 2012.

31. K. Danas, P. Ponte Castañeda. *Influence of the Lode parameter and the stress triaxiality on the failure of elasto-plastic porous materials*. **International Journal of Solids and Structures, 49**, 1325-1342, 2012.

32. A. Ridruejo, C. González, J. LLorca. *A constitutive model for the in-plane mechanical behavior of nonwoven fabrics*. **International Journal of Solids and Structures, 49**, 2215–2229, 2012.

33. O. López-Pamies, P. Ponte Castañeda, M. Idiart. *Effects of internal pore pressure on closed-cell elastomeric foams*. **International Journal of Solids and Structures, 49**, 2793-2798, 2012.

34. M. I. Martín, F. A. López, J. M. Torralba. *Production of sponge iron powder by reduction of rolling mill scale*. **Ironmaking & Steelmaking, 39**, 155-162, 2012.

35. R. Z. Valiev, I. Sabirov, A. P. Zhilyaev, T. G. Langdon. *Bulk Nanostructured Metals for Innovative Applications*. **JOM, 64**, 1134-1142, 2012.

36. I. Martin-Bragado, B. Sklenard. *Understanding Si(111) solid phase epitaxial regrowth using Monte Carlo modeling: Bi-modal growth, defect formation, and interface topology*. **Journal of Applied Physics, 112**, 024327-024331, 2012.

37. E. Lorenzo-Villafranca, K. Tamargo-Martínez, J. M. Molina-Aldareguia, C. González, A. Martínez-Alonso, J. M. D. Tascón, M. Gracia, J. LLorca. *Influence of plasma surface treatments on kink band formation in PBO fibers during compression*. **Journal of Applied Polymer Science, 123**, 2052-2063, 2012.

38. K. Raghu Raja Pandiyan, N. Swati. *Viscosity modeling of a medium reactive unsaturated polyester resin used for liquid composite molding process*. **Journal of Applied Polymer Science, 125**, 1400-1408, 2012.

39. O. López-Pamies, J. Moraleda, J. Segurado, J. LLorca. *On the Extremal Properties of Hashin's Hollow Cylinder Assemblage in Nonlinear Elasticity*. **Journal of Elasticity, 107**, 1-10, 2012.

40. A. Dasari, J. Quirós, B. Herrero, K. Boltes, E. García-Calvo, R. Rosal. *Antifouling membranes prepared by electrospinning polylactic acid containing biocidal nanoparticles*. **Journal of Membrane Science, 405**, 134-140, 2012.

41. P. Ponte Castañeda. *Bounds for nonlinear composites via iterated homogenization*. **Journal of the Mechanics and Physics of Solids, 60**, 1583-1604, 2012.

42. J. Hidalgo, A. Jiménez-Morales, J. M. Torralba. *Torque rheology of zircon feedstocks for powder injection moulding*. **Journal of the European Ceramic Society, 32**, 4063–4072, 2012.

43. D. Y. Wang, U. Gohs, N. J. Kang, A. Leuteritz, R. Boldt, U. Wagenknecht, G. Heinrich. *Method for simultaneousiy improving the thermal stability and mechanical properties of Poly(Lactic Acid): effect of high-energy electrons on the morphological, mechanical, and thermal properties of PLA/MMT nanocomposites*. **Langmuir, 28**, 12601-12608, 2012.

44. N. V. Dudamell, I. Ulacia, F. Gálvez, S. Yi, J. Bohlen, D. Letzig, I. Hurtado, M. T. Pérez-Prado. *Influence of texture on the recrystallization mechanisms in an AZ31 Mg sheet alloy at dynamic rates*. **Materials Science and Engineering A, 532**, 528-535, 2012.

45. M. A. Jabbari Taleghani, E. M. Ruiz Navas, M. Salehic, J. M. Torralba. *Hot deformation behaviour and flow stress prediction of 7075 aluminium alloy powder compacts during compression at elevated temperatures*. **Materials Science and Engineering A, 534**, 624– 631, 2012.

46. J. J. Williams, J. Segurado, J. LLorca, N. Chawla. *Three dimensional (3D) microstructure-based modeling of interfacial decohesion in particle reinforced metal matrix composites*. **Materials Science and Engineering A, 557**, 113–118, 2012.

47. R. Muñoz-Moreno, C. J. Boehlert, M. T. Pérez-Prado, E. M. Ruiz-Navas, J. LLorca. *In situ observations of the deformation behavior and fracture mechanisms of Ti-45Al-2Nb-2Mn + 0.8 vol pct TiB2*. **Metallurgical and Materials Transactions, 43A**, 1198-2018, 2012.

48. B. Tang, Y.-W. Cui, H. Chang, H. Kou, J. Li, L. Zhou. *Modeling of Incommensurate ω Structure in the Zr-Nb Alloys*. **Metallurgical and Materials Transactions A, 43**, 2581-2586, 2012.

49. B. Galiana, M. Benedicto, L. Vázquez, J. M. Molina-Aldareguia, P. Tejedor. *Thermal stability of HfO2-on-GaAs nanopatterns*. **Nanoscale, 4**, 3734-3738, 2012.

50. M. Agoras, P. Ponte Castañeda. *Multi-scale homogenization-based modeling of semi-crystalline polymers*. **Philosophical Magazine, 92**, 925-958, 2012.

51. D. Edwards, I. Sabirov, W. Sigle, R. Pippan. *Microstructure and thermostability of a W–Cu nanocomposite produced via high-pressure torsion*. **Philosophical Magazine, 92**, 4151-4166, 2012.

52. S. Lotfian, J. M. Molina-Aldareguía, K. E. Yazzie, J. LLorca, N. Chawla. *High temperature nanoindentation behavior of Al/SiC multilayers*. **Philosophical Magazine Letters, 92**, 362-367, 2012.

53. T. Gao, H. H. Hu, P. Ponte Castaneda. *Shape Dynamics and Rheology of Soft Elastic Particles in a Shear Flow*. **Physical Review Letters, 108**, 058302, 2012.

54. S. Drensler, C. Cela Mardare, S. Milenkovic, A. Walter Hassel. *Selective dissolution in AlFeNb alloys*. **Physica Status Solidi A, 209**, 854-858, 2012.

55. F. Cervantes-Sodi, A. Íñiguez-Rábago, S. Rosas-Meléndez, M. Ballesteros-Villarreal, Juan J. Vilatela, L. G. Reyes-Gutiérrez, E. Palacios, M. Terrones, Jose A. Jiménez-Rodríguez. *Selective synthesis of double hélices of carbon nanotube bundles grown on treated metallic substrates*. **Physica Status Solidi B**, **249**, 2382–238, 2012.

56. J. A. González, A. Dasari, B. Herrero, E. Plancher, J. Santarén, A. Esteban, S.-H. Lim. *Fire retardancy behavior of PLA based nanocomposites*. **Polymer Degradation and Stability, 97**, 248-256, 2012.

57. K. Raghu Raja Pandiyan, V. M. Shinde, S. Neogi. *Measurement of effective permeability of reinforcement mats using sensitivity analysis*. **Polymer Composites, 33**, 1445-1454, 2012.

58. E. Bernardo, J. Hidalgo, A. Jiménez-Morales, J. M. Torralba. *Feedstock development for powder injection moulding of Zirconium Silicate*. **Powder Injection Moulding International, 6**, 75-78, 2012.

59. M. A. Jabbari Taleghani, E. M. Ruiz Navas, M. Salehi, J. M. Torralba. *Optimisation of mechanical milling process for production of AA 7075/(SiC or TiB2) composite powders*. **Powder Metallurgy, 55**, 280-286, 2012.

60. R. Oro, M. Campos, J. M. Torralba, C. Capdevila. *Lean alloys in PM: from design to sintering Performance*. **Powder Metallurgy, 55**, 294-301, 2012.

61. A. T. Sepúlveda, R. Guzmán de Villoria, J. C. Viana, A. J. Pontes, B. L. Wardle, L. A. Rocha. *Flexible Pressure Sensors: Modeling and Experimental Characterisation*. **Procedia Engineering, 47**, 1177-1180, 2012.

62. A. Jérusalem, A. Fernández, A. Kunz, J. R. Greer. *Continuum modeling of dislocation starvation and subsequent nucleation in nano-pillar compression*. **Scripta Materialia, 66**, 93-96, 2012.

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

64. C. S. Wong, N. S. Bennett, B. Galiana, P. Tejedor, M. Benedicto, J. M. Molina-Aldareguia, P. J. McNally. *Structural investigation of MOVPE-grown GaAs on Ge by x-ray techniques*. **Semiconductor Science and Technology, 27**, 115012, 2012.

65. L. A. Fasce, R. Seltzer, P. M. Frontini. *Depth sensing indentation of organic-inorganic hybrid coatings deposited onto a polymeric substrate*. **Surface & Coatings Technology, 210**, 62–70, 2012

6.2. Book Chapters

1. J. M. Torralba. *Metal injection molding (MIM) of stainless steel*, in **Handbook of Metal Injection Molding**, Edited by Donald F. Heaney, Woodhead Publishing, 393-414, 2012.

2. M. H. Doweidar, R. M. Sánchez, E. Peña, B. Calvo and M. Doblaré. Chapter 2. 3D *Computational Modeling of the Human Knee in Physiological state,* in **The Knee: Current Concepts in Kinematics, Injury Types, and Treatment Options**, Randy Mascarenhas, University of Manitoba, Canada, 2012.

3. R. Muñoz, R. Seltzer, F. Sket, C. González, J. LLorca. *Mechanical charaterisation of 3D woven materials against impact loads.* **15th European Conference on Composite Materials**, 2012.

4. S. Hernandez, F. Sket, C. González, J. M. Molina-Aldareguía, J. LLorca. *Analysis of curing cycle on processing void distribution and mechanical properties of a polymer composite material.* **15th European Conference on Composite Materials**, 2012.

5. F. Sket, A. Enfedaque, C. Alton, S. Sádaba, J. M. Molina-Aldareguía, C. González, J. LLorca. *Detailed damage mechanisms assessment in composite materials by means of X-ray tomography.* **15th European Conference on Composite Materials**, 2012.

6. M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca. *Micromechanical modeling of the effect of hot-wet conditions on the mechanical behavior of composite materials.* **15th European Conference on Composite Materials**, 2012.

7. C. J. Davidson, T. R. Finlayson, J. R. Griffiths, V. Luzin, Q. G. Wang, J. Rajakesari, J. LLorca. *Neutron Diffraction Determination of Macro and Microstresses in an Al-Si-Mg Composite and Observed Changes with Plastic Strain.* **36th Australian Annual Condensed Matter and Materials Meeting**, 2012.

6.3. Patents

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

2. *"Method to obtain the beta phase of a transition pure metal of the group IV of the periodic system and product resulting from this method"*. M. T. Pérez-Prado, A. P Zhilyaev, A. Sharafutdinov. Patent ES2347117 (Spain) and PCT/ES2010/070017.

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

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

book chapters

patents

6.4. International Congresses

6.4.1. Invited and Plenary Talks

1. *"Simulation of size effects in the growth of cylindrical voids by means of dislocation dynamics and molecular dynamics"*. J. Segurado, H.-J. Chang, O. Rodriguez, B. Martínez J. LLorca, **International Symposium on Plasticity**, San Juan, Puerto Rico, January, 2012.

2. *"Simulation of size effects in 2D void growth by means of dislocation dynamics and molecular dynamics"*. J. Segurado. **International Symposium on Plasticity**, San Juan, Puerto Rico, January 2012.

3. *"Bounds of the Hashin-Shtrikman type for nonlinear magneto-elastic composites."* P. Ponte-Castañeda. **Symposium on Micromechanics of Composite Materials** (in honor of Professor Zvi Hashin on the occasion of the award of the Franklin Medal), Villanova University, PA, US, April 2012.

4. *"Multiscale modeling of composites: a roadmap towards virtual testing"*, J. LLorca. **Materials Genome Initiative Forum**, Shanghai University, Shanghai, China, May 2012.

5. *"Integrated computational alloy design for advanced rare metal materials: Thermo-kinetic modeling & phase field approach"*. Y. Cui. **Material Genome Initiative Forum,** Shanghai, China, May 2012.

6. *"Virtual testing of composites: roadmap, lessons learned and necessary breakthroughs"*, J. LLorca, **Workshop on the Design of Ceramic–Fiber Based Composites for Service Above 1400ºC**, Boulder, Colorado, US, June 2012.

7. *"Modeling and optimization of solar cells"*, V. Moroz, J. Huang, G. Letay, I. Martin-Bragado. I. Martin-Bragado. **12th Ion Implant Technology**, Valladolid, Spain, June 2012.

8. *"Fracture of heterogeneous materials: a microstructural perspective"*. J. LLorca, L. P. Canal, C. González, J. Segurado, J. M. Molina-Aldareguía, F. Sket. **IUTAM Symposium on Fracture Phenomena in Nature and Technology**, Brescia, Italy, July 2012.

9. *"The effect of porosity and its anisotropic evolution on the viscoplastic behavior of metals"*. P. Ponte-Castañeda. **IUTAM Symposium on Fracture Phenomena in Nature and Technology**, Brescia, Italy, July 2012.

10. "*Effect of tilt on the micropillar compression of LiF single crystals"*. J.M. Molina-Aldareguia, R. Soler, J Segurado, J. LLorca. **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

11. *"Non-Conventional laminates: Expanding the design envelope and improving the structural performance of advanced composites"*, C. S. Lopes, Z. Gürdal, P. P. Camanho, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

12. *"High Temperature nanoindentation behavior of Al/SiC nanoscale multilayers"*. J. M. Molina-Aldareguia, S. Lotfian, K. Yazzie, N. Chawla, J. LLorca. **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, July 2012.

13. *"Constitutive models for magneto-elastic composites at finite strains: The effects of particle shape and anisotropy"*. P. Ponte-Castañeda. **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

14. *"Oxidation behavior and thermal stability of a NiAl-V alloy"*. S. Milenkovic, R. Caram. **Engineering of Functional Interfaces, EnFI 2012**, Zweibrücken, Germany, July 2012.

15. *"3D pattern control of templatelessly grown monocrystalline Mo nanowire arrays"*. S. Milenkovic, A. W. Hassel. **Electrochemistry of Micro and Nano Technology, EMNT 2012**, Linz, Austria, August 2012.

16. *"Multiscale modelling of composites: a roadmap towards virtual testing"*. J. LLorca. **XXII International Workshop on Computational Mechanics of Material**, Baltimore, Maryland, US, September 2012.

17. *"Nanoscale metallic and metal-ceramic multilaters for radiation-resistant applications"*. S. Lotfian, M. Rodríguez, M. Monclús, J. M. Molina-Aldareguía, J. LLorca. **Trends in NanoTechnology, TNT2012**, Madrid, Spain, September 2012.

18. *"An innovative method for high-throughput investigation of the solidification-microstructure relationships"*. S. Milenkovic, I. Sabirov, J. LLorca. **Advanced Materials and Processing Technologies, AMPT 2012**, Wollongong, Australia, September 2012.

19. *"Development of high performance powder metallurgy steels by high energy milling"*. J. M. Torralba, L. Fuentes-Pacheco, N. García-Rodriguez, M. Campos. **4th International Conference on the Characterisation and Control of Interfaces for High Quality Advanced Material,** Kurashiki, Japan, September 2012.

20. *"Phase transformations in metals by high pressure torsion"*. M. T. Pérez-Prado, A. P. Zhilyaev, B. Srinivasarao. **EMRS Fall meeting**, Warsaw, Poland, September 2012.

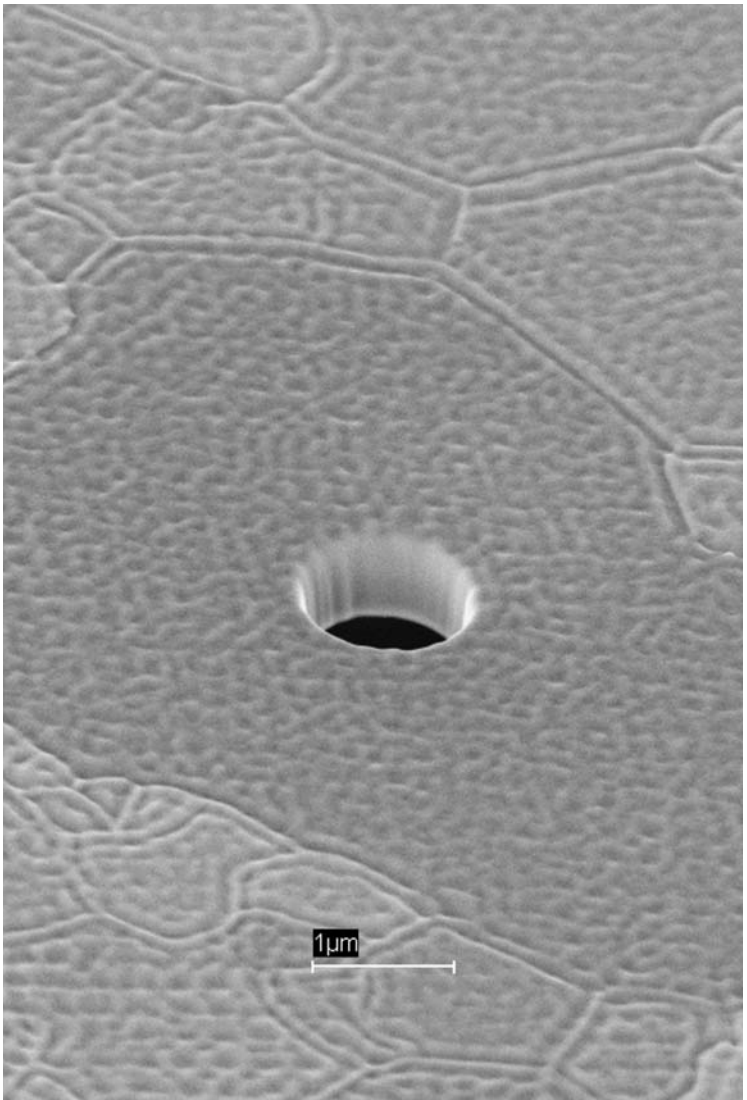
21. *"EBSD study of the evolution of the microstructure of a Mg alloy under dynamic conditions"*. M. T. Pérez-Prado, N. Dudamell, F. Gálvez, S. Yi, J. Bohlen, D. Letzig. International symposium on hot plastic deformation and texture analysis. **Spanish National Conference on Mechanical Properties of Solids, PMS 2012**, Alcoy, Spain, September 2012.

22. *"Multiscale modeling of fracture in composites: a roadmap towards virtual testing"*. J. LLorca, C. González, J. M. Molina-Aldareguia, J. Segurado. **49th Annual Technical Meeting, Society of Engineering Science**, Atlanta, Georgia, US, October 2012.

23. *"Microstructure evolution and its effect on the macroscopic response and stability of porous metals"*. P. Ponte-Castañeda. **49th Annual Technical Conference of the Society of Engineering Science**, Georgia Tech, US, October 2012.

24. *"Integrated alloy design for advanced metal materials"*. Y. Cui, **International Symposium on Phase Diagram and Alloy Design**, Changzhou, China, October 2012.

25. *"Optimization of the mechanical behavior of composites under impact by means of multiscale modeling*". C. S. Lópes, C. González, J. LLorca. **Materials Research Society Fall Meeting**, Boston, Massachusetts, US, November 2012.



6.4.2. Regular Contributions

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

2. *"Multifunctional composites based on nanocarbons"*. J. J. Vilatela, B. Mas, J. P. Fernández-Blázquez, M. Monclús, J. Molina. **NanoSpain 2012**, Santander, Spain, February 2012.

3. *"Tip shape effect on the hot indentation hardness and modulus of Al and SiC*". M. A. Monclus, S. Lotfian, J. Molina-Aldareguia. **Nanomechanical Testing Workshop, Nanobrücken II**, Saarbrücken, Germany, March 2012.

4. *"Tensile and creep deformation mechanisms in rolled AZ31"*. C. J. Boehlert, Z. Chen, I. Gutiérrez-Urrutia, J. Bohlen, S. Yi, D. Letzig, J. LLorca, M. T. Pérez-Prado. **2012 TMS Annual Meeting & Exhibition**, Orlando, Florida, USA, March 2012.

5. *"Mechanical characterisation of nanolayered Al/SiC composites by high temperature nanoindentation"*. S. Lotfian, J. M. Molina-Aldareguia, K. Yazzie, J. LLorca, A. Misra, N. Chawla. **2012 TMS Annual Meeting & Exhibition**, Orlando, Florida, USA, March 2012.

6. *"FDSOI devices: A solution to achieve low junction leakage with low temperature processes (< 650° C)"*. B. Sklenard, C. Xu, P. Batude, B. Previtali, C. Tabone, Q. Rafhay, B. Colombeau, F. A. Khaja, I. Martin-Bragado, J. Berthoz. **13th ULIS: Ultimate Integration on Silicon**, Grenoble, France, March 2012.

7. *"In-situ analysis of the deformation mechanisms in Mg alloys between 50-250°C"*. Z. Chen, A. Chakkedath, I. Gutiérrez-Urrutia, J. Bohlen, S. Yi, D. Letzig, J. LLorca, M. T. Pérez-Prado, C. J. Boehlert. **TMS 2012 Annual Meeting and Exhibition**, Orlando, Florida, USA, March 2012.

8. *"In-plane stiffness tailoring for the improvement of buckling and strength of composite panels with cut-outs"*. C. S. Lopes, Z. Gürdal, P. P. Camanho, V. S. Gomes. **European Conference on Spacecraft Structures, Materials & Environmental Testing**, ESA/ESTEC, Noordwijk, The Netherlands, March 2012.

9. *"Optimization of dispersed laminates for aircraft structures"*. T. A. Sebaey, J. Costa, C. S. Lopes, N. Blanco. **SAMPE Europe Student Conference 2012**, Paris, France, March 2012.

10. *"Aligned carbon nanotube reinforcement of aerospace carbon fiber composites: substructural strength evaluation for aerostructure applications"*. R. Guzmán de Villoria, L. Ydrefors, P. Hallander , K. Ishiguro, P. Nordin, B. L. Wardle. **53rd AIAA Structures, Structural Dynamics, and Materials Conference**, **AIAA-2012-1566**, Honolulu, Hawaii, USA, April 2012.

11. *"Elastic properties of aligned carbon nanotube polymer nanocomposites with controlled morphology"*. D. Handlin, R. Guzmán de Villoria, S. H. Chan, K. Takahashi, H. Cebeci, M. Williams, E. M. Parsons, S. Socrate, B. L. Wardle. **53rd AIAA Structures, Structural Dynamics, and Materials Conference**, **AIAA-2012-1565**, Honolulu, Hawaii, USA, April 2012.

12. *"Effective stiffness of wavy aligned carbon nanotubes for modeling of controlled-morphology polymer nanocomposites"*. H. Cebeci, R. Guzmán de Villoria, R. M. Jones, K. Schulte, H. S. Türkmen, B. L. Wardle. **53rd AIAA Structures, Structural Dynamics, and Materials Conference**, **AIAA-2012-1565**, Honolulu, Hawaii, USA, April 2012.

13. *"Tomographic investigation of creep damage in P91 and E911 steels"*. F. Sket, K. Maile, H. Ruoff, R. Scheck, A. Borbely. **12th International Conference on Creep and Fracture of Engineering Materials and Structures, Creep 2012 / JIMIS 11**, Kyoto, Japan, May 2012.

14. *"Improving the structural performance of advanced composites with nonconventional laminates"*. C. S. Lopes, Z. Gürdal, P. P. Camanho, T. Sebaey. **XVII International Conference Mechanics Of Composite Materials**, Riga, Latvia, May 2012.

15. *"Structure and properties of composites of carbon nanotube fibres"*. J. J. Vilatela, R. Khare, A. H. Windle. **15th European Conference on Composite Materials**, Venice, Italy, June 2012.

16. *"Mechanical characterisation of 3D woven materials against impact loads"*. R. Muñoz, R. Seltzer, F. Sket, C. González, J. LLorca. **15th European Conference on Composite Materials**, Venice, Italy, June 2012.

17. *"Analysis of curing cycle on processing void distribution and mechanical properties of a polymer composite material"*. S. Hernandez, F. Sket, C. González, J. M. Molina-Aldareguía, J. LLorca. **15th European Conference on Composite Materials**, Venice, Italy, June 2012.

18. *"Detailed damage mechanisms assessment in composite materials by means of X-ray tomography"*. F. Sket, A. Enfedaque, C. Alton, S. Sádaba, J. M. Molina-Aldareguía, C. González, J. LLorca. **15th European Conference on Composite Materials**, Venice, Italy, June 2012.

19. *"Micromechanical modeling of the effect of hot-wet conditions on the mechanical behavior of composite materials"*. M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca. **15th European Conference on Composite Materials**, Venice, Italy, June 2012.

20. *"On the controversy of grain boundary sliding in Mg AZ31"*. C. Boehlert, Z. Chen, I. Gutiérrez-Urrutia, J. LLorca, M. T. Pérez-Prado. **International Conference on Superplasticity of Advanced Materials, ICSAM 2012**, Albi, France, June 2012.

21. *"MMonCa: A flexible and powerful new Kinetic Monte Carlo simulator"*. I. Martin-Bragado, A. Rivera, G. Valles, M. J. Caturla. **2012 COSIRES**, Santa Fe, New Mexico, USA June 2012.

22. *"Effect of ion flux on helium retention in helium-irradiated tungsten"*. A. Rivera, G. Valles, M. J. Caturla, I. Martin-Bragado. **2012 COSIRES**, Santa Fe, New Mexico, USA June 2012.

23. *"A phase-field approach to athermal , ? ˆ phase transformation and its pre-transition effect of Zr-Nb alloys"*. Y.-W. Cui, B. Tang. **CALPHAD XLI**, Berkeley, California, USA, June 2012.

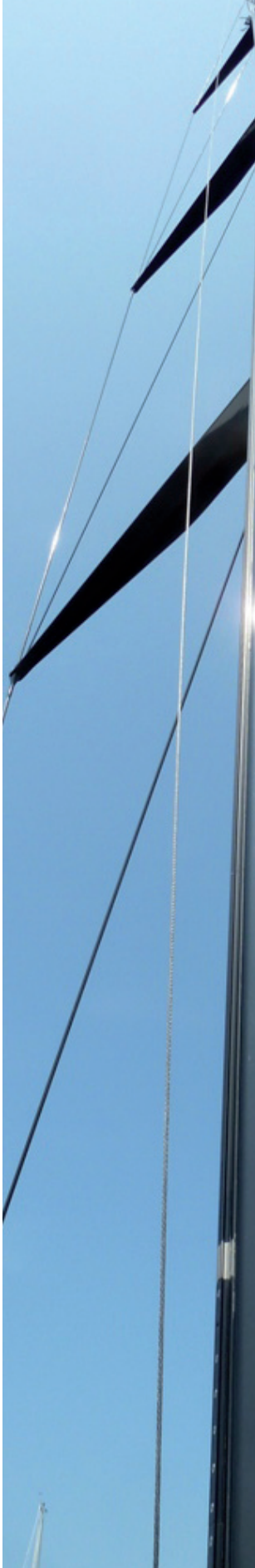
24. *"Effect of tilt on the micropillar compression of plastically anisotropic single-crystals"*. R. Soler, J. M. Molina-Aldareguia, J. Segurado, J. LLorca. Symposium on Experimental Micromechanics and Nanomechanics, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

25. *"High temperature nanoindentation behavior of Al/SiC nanoscale multilayers"*. S. Lotfian, J. M. Molina-Aldareguía, K. E. Yazzie, J. LLorca, N. Chawla. Symposium on Mechanics of Nanoindentation, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

26. *"A constitutive model for the tensile behavior of nonwovens"*. A. Ridruejo, C. González, J. LLorca. Symposium on Mechanics of Textile Composite Reinforcements, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

27. *"Multiscale modeling of acumulative roll bonding (ARB) process"*. J. Segurado, A. Ridruejo, J. LLorca. Symposium on Multiscale Modelling of Polycrystalline Plasticity, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

28. *"Micromechanical study of the failure of fiber-reinforced polymers"*. L. P. Canal, C. González, J. Segurado, J. LLorca. Symposium on Virtual Testing of Composites, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.



29. *"Modelling of the low-velocity impact behaviour of 3D orthogonal hybrid woven composites"*. R. Muñoz, R. Seltzer, F. Martínez, C. González, J. LLorca. Symposium on Virtual Testing of Composites, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

30. *"Determination of the mechanical properties of amorphous materials through instrumented indentation"*. M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca. General Session on Material Mechanics, **8th European Solids Mechanics Conference**, **ESMC 2012**, Graz, Austria, July 2012.

31. *"Influence of hydrostatic pressure on porosity of die-cast Mg alloys: experimental and numerical studies"*. A. Fernández, F. Sket, J. Molina, M.T. Pérez-Prado, A. Jérusalem. **8th European Solid Mechanics Conference, ESMC 2012**, Graz, Austria, 2012.

32. *"Influence of hydrostatic pressure on porosity of die-cast Mg alloys: experimental and numerical studies"*. A. Fernández, F. Sket, A. Jerusalem, J. Molina-Aldareguia, T. Pérez-Prado. **8th European Solid Mechanics Conference, ESMC 2012**, Graz, Austria, July 2012.

33. *"Microstructure-mechanical property correlation on high pressure die cast AZ91 Mg alloy"*. S. Biswas, F. Sket, M .T. Pérez-Prado. **International Conference on Strength of Materials, ICSMA 2012**, Bangalore, India, August 2012.

34. *"Effect of microstructure on mechanisms for plastic flow in ultra-fine grained Al-Mg-Si alloy"*. I. Sabirov, M. Yu. Murashkin, V. U. Kazykhanov, R.Z. Valiev. **EMRS 2012 Fall Meeting**, Warsaw, Poland, September 2012.

35. *"Liquid phase sintering control based on effective alloying design"*. R. Oro, E. Bernardo, M. Campos y J. M. Torralba. **Euro PM'2012**, Basel, Switzerland, September 2012.

36. *"Effect of liquid content on dimensional stability and sinter properties of liquid-phase sintered low alloyed steels"*. E. Bernardo, R. Oro, M. Campos, R. Frykholm, O. Litström, J. M. Torralba**. Euro PM'2012**, Basel, Switzerland, September 2012.

37. *"Multifunctional composites based on nanocarbons"*. J. J. Vilatela. **International Workshop on Nanocarbon Composites**, Valencia, Spain, October 2012.

38. *"High temperature micropillar compression of LiF single crystals*. J. M. Molina-Aldareguia, R. Soler, J Segurado, J. LLorca. **49th Annual Meeting of the Society of Engineering Sciences, SES 2012,** Atlanta, USA, October 2012.

39. *"Simulation of size effects in the growth of cylindrical voids by means of dislocation dynamics and molecular dynamics"*. J. Segurado, J. LLorca, H.-J. Chang, O. Rodríguez. **49th Annual Meeting of the Society of Engineering Sciences, SES 2012**, Atlanta, Georgia, October 2012.

40. *"Micropillar compression of LiF between room temperature and 400ºC"*. J. M. Molina-Aldareguia, R. Soler, J. Wheeler, J. Segurado, J. Michler, J. LLorca. **49th Annual Meeting of the Society of Engineering Sciences, SES 2012**, Atlanta, Georgia, October 2012.

41. *"High temperature mechanical behaviour of nanoscale multilayers"*. J. M. Molina-Aldareguia, M. Monclus, S. Lotfian, K. Yazzie, J. LLorca, N. Chawla, N. Mara, I. Beyerlein. **49th Annual Meeting of the Society of Engineering Sciences, SES 2012**, Atlanta, Georgia, October 2012.

42. *"Damage tolerance of non-conventional laminates with dispersed stacking sequences"*, C. S. Lopes, T. Sebaey. **6th International Symposium on Manufacturing Technology for Composite Aircraft Structures**, Stade, Germany, October 2012.

43. *"High temperature mechanical properties of Al/SiC and Cu/Nb nanoscale multilayers"*. M. A. Monclus, S. Lotfian, J. Molina-Aldareguia. **12th European Nanomechanical User Group Meeting**, Valletta, Malta, October 2012.

44. *"Discrete (MD) and continuum (DD) simulations of void growth in single crystals*". H.-J. Chang, J. Segurado, J. LLorca, O. Rodríguez. **6th International Conference on Multiscale Modelling of Materials**, Singapore, October 2012.

45. *"On the macroscopic response of deformable dielectric composites and applications to electrostriction"*. P. Ponte-Castañeda, M. Hakimi-Siboni. **49th Annual Technical Conference of the Society of Engineering Science**, Atlanta, Georgia, USA, October 2012.

46. *"Constitutive models for magneto-elastic composites at finite strains: the effects of particle rotations and magnetic torques"*. P. Ponte-Castañeda, E. Galipeau. **49th Annual Technical Conference of the Society of Engineering Science**, Atlanta, Georgia, USA, October 2012.

47. *"In situ analysis of the deformation & fracture mechanisms of Ti-45Al-2Nb-2Mn-0.8v.%TiB_2 at high temperature"*. R. Muñoz-Moreno, C. J. Boehlert, M. T. Pérez-Prado, E. M. Ruiz-Navas, J. LLorca. **Materials Research Society Fall Meeting**, Boston, Massachusetts, November 2012.

48. *"High temperature mechanical properties of Cu/Nb nanoscale multilayers"*. M. Monclús, J. M. Molina-Aldareguía, J. LLorca. **Materials Research Society Fall Meeting**, Boston, Massachusetts, November 2012.

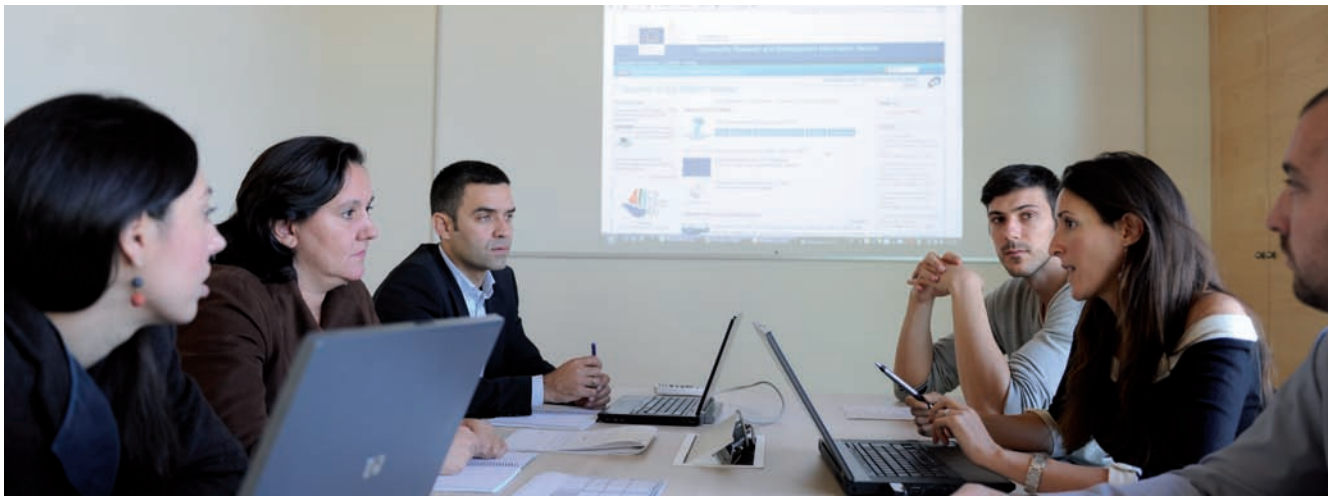
49. *"A novel methodology to determine the mechanical properties of amorphous materials through instrumented nanoindentation"*. M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca. **Materials Research Society Fall Meeting**, Boston, Massachusetts, November 2012.

50. *"Defect Evolution under continuous and pulsed helium irradiation of tungsten: relevance for armor applications in laser fusion reactors"*. A. Rivera, G. Valles, M. J. Caturla, I. Martin-Bragado. **Materials Research Society Fall Meeting**, Boston, Massachusetts, USA, November 2012.

51. *"Elastomeric solids with pressurized cavities: From defects to closed-cell foams"*. P. Ponte-Castañeda, O. Lopez-Pamies, **ASME International Mechanical Engineering Congress and Exposition**, Houston, Texas, November 2012.

52. *"Constitutive models for magneto-elastic composites at finite strains: The effects of particle rotations and magnetic torques"*. P. Ponte-Castañeda, E. Galipeau. **ASME International Mechanical Engineering Congress and Exposition**, Houston, Texas, November 2012.

53. *"Massively parallel implementation of XFEM for fracture simulations"*. D .D. Tjahjanto, C. Samaniego, G. Houzeaux, M. Vázquez, A. Jérusalem. **ABAQUS workshop on Modelling Fracture and Failure**, Oxford, UK, November 2012.



6.5. Invited Seminars and Lectures

1. *"Atomistic modeling for the anisotropic SPER and defect formation in Silicon"*. I. Martin-Bragado. **Synopsys Inc.**, Zurich, Switzerland, February 2012.

2. *"Coupling cell mechanics, cell damage, and electrophysiological functions in neurons"*. A. Jérusalem. Department of Mechanical Engineering, **École Polytechnique Fédérale de Lausanne**, Lausanne, Switzerland, February 2012.

3. *"On the quest of engineering ceramics for very high temperature structural applications"*. J. LLorca. **Shanghai Institute of Ceramics, Chinese Academy of Sciences**, Shanghai, China, May 2012.

4. *"Multiscale modelling of composites: a roadmap for virtual testing"*. J. LLorca. State Key Laboratory for Metal-Matrix composites. **Shanghai Jiao Tong University**, Shanghai, China, May 2012.

5. *"Multiscale modelling of engineering materials"*. J. LLorca. School of Materials Science and Engineering. **University of Science and Technology of Beijing**, Bejing, China, May 2012.

6. *"Multiscale modelling of composites: a roadmap for virtual testing"*. J. LLorca. **Institute of Mechanics, Chinese Academy of Sciences,** Beijing, China, May 2012.

7. *"Computational neuroscience simulations: Synaptic tansmission, cell mechanics and functions in neurons"*. A. Jérusalem, J. M. Peña. Laboratorio de Circuitos Corticales (CTB), **Polytechnic University of Madrid**, Madrid, Spain, May 2012.

8. *"Plastic deformation at high temperature at the micrometer and nanometer scale"*. J. LLorca. **Los Alamos National Laboratory**, Los Alamos, New Mexico, June 2012.

9. *"Atomistic modeling for the anisotropic SPER and defect formation in Silicon"*. I. Martin-Bragado. **Synopsys Inc.**, Mountain View, CA, USA, June 2012.

10. *"Extending KMC to metals"*. I. Martin-Bragado. **Synopsys Inc.**, Mountain View, CA, USA, June 2012.

11. "Simulation of plastic behavior at different length scales: from the nano- to the macro-scale". J. Segurado. Institute of Lightweight Design and Structural Biomechanics, **Vienna University of Technology**, Vienna, Austria, July 2012.

12. *"Defect diffusion modeling: Kinetic Monte Carlo"*. I. Martin-Bragado. **Polytechnic University Summer School**, La Granja, Spain, July 2012.

13. *"Multifunctional composites based on nanocarbons"*. J. J. Vilatela. Department of Materials Science and Metallurgy. **University of Cambridge**, Cambridge, UK, September 2012.

14. *"Multiscale modelling of composites: a roadmap for virtual testing"*. J. LLorca. School of Civil and Environmental Engineering. **Cornell University,** Ithaca, New York, September 2012.

15. *"Plastic deformation at high temperature at the micrometer and nanometer scale"*. J. LLorca. Department of Mechanical and Aerospace Engineering. **Rutgers University**, Piscataway, New Jersey, September 2012.

16. *"Diffusion research and computational diffusion kinetics"*. Y. Cui. School of Materials Science and Engineering, **Shanghai University**, Shanghai, China, September 2012.

17. *"From powders to high performance alloys and metal matrix composites"*. J. M. Torralba. Joining and Welding Research Institute, **Osaka University**, Japan, September 2012.

18. *"High temperature mechanical properties of nanoscale multilayers"*. J. M. Molina-Aldareguia. **Arizona State University**, Tempe, October 2012.

19. *"High temperature nanomechanics"*. J. LLorca. Materials Science and Technology Division. **Oak Ridge National Laboratory**, Oak Ridge, Tennessee, October 2012.

20. *"Front-end process modeling in silicon: Kinetic Monte Carlo (KMC) approaches"*. I. Martin-Bragado. **CEA-LETI**, Grenoble, France, October 2012.

21. *"Integrated computational alloy design for rare metal materials: thermo-kinetic modeling & phase field approach"*. Y. Cui. School of Materials Science and Engineering, **Northwestern Polytechnical University**, Xi'an, China, November 2012.

22. *"Integrated studies of advanced Ti alloys: thermodynamics, diffusion kinetics and microstructure"*, Y. Cui, School of Materials Science and Engineering, **Central South University**, Changsha, China, November 2012.

23. *"Integrated alloy design for Ti and Zr alloys"*. Y. Cui. Institute of Materials Research, **Shanghai University**, Shanghai, China, November 2012.

24. *"High performance environmentally friendly polymer nanocomposites"*. D. Y. Wang. **Federal Institute for Materials Research and Testing**, Berlin, Germany, December 2012.

6.6. Organization of Conferences, Workshops and Courses

1. **12th International Workshop on Stress-Induced Phenomena in Metallization**. J. Molina-Aldareguia (Member of the Scientific Committee). Kyoto, Japan, May 2012.

2. **SIAM Conference on Mathematical Aspects of Materials Science**. P. Ponte-Castañeda, (Symposium Organizer on Homogenization and Applications). Philadelphia, Pennsylvania, USA, June 2013.

3. **European Powder Metallurgy Association PM Summer School**. J. M. Torralba (Academic Coordinator and Organizer). San Sebastian, Spain, June 2012.

4. **IV Spanish Powder Metallurgy Congress**. J. M. Torralba (Honorary Chairman and member of the Scientific Committee). Seville, Spain, June 2012.

5. **XII National Congress on Materials**. J. M. Torralba (Scientific Committee Member). Alicante, Spain, June 2012.

6. **International Conference on High Performance Computing & Simulation**, **HPCS 2012.** A. Jérusalem (Poster Co-chair). Madrid, Spain, July 2012.

7. **International Symposium on Hot Plastic Deformation and Texture Analysis**. M. T. Perez-Prado (Member of the Scientific Committee). Alcoy, Spain, July 2012.

conferences workshops courses

8. **8th European Solid Mechanics Conference, ESMC 2012**. J. LLorca. (Symposium Co-organizer on Advanced Composite Materials). Graz, Austria, July 2012.

9. **8th European Solid Mechanics Conference, ESMC 2012**. J. Segurado (Symposium Co-Organizer on Multiscale Modelling of Polycrystalline Plasticity). Graz, Austria, July 2012.

10. **8th European Solid Mechanics Conference, ESMC 2012**. C. González (Symposium Co-Organizer on Virtual Testing of Composites). Graz, Austria, July 2012.

11. **8th European Solid Mechanics Conference, ESMC 2012**. J. Molina-Aldareguia (Symposium co-organizer on Experimental Micro and Nanomechanics). Graz, Austria, July 2012.

12. **11th International Conference on Superplasticity in Advanced Materials, ICSAM 2012**. M. T. Perez-Prado (International Advisory Board). Albi, France, July 2012.

13. **15th International Conference on Strength of Materials, ICSMA 2012**, M. T. Perez-Prado (International Advisory Board). Bangalore, India, August 2012.

14. **European Powder Metallurgy Congress, EUROPM 2012**. J. M. Torralba (Technical Programme Committee). Basel, Switzerland, September 2012.

15. **4th International Conference on the Characterisation and Control of Interfaces for High Quality Advanced Materials**. J. M. Torralba (Scientific Committee Member). Kurashiki, Japan, September 2012.

6.7. Seminars

1. *"New developments in the processing and properties of ultrafine-grained metals".* **Prof. T. G. Langdon** (from University of Southampton, UK and University of Sothern California, Los Angeles, Californmia, USA). May 2012.

2. *"Hot spots in viscoplastic deformation of polycristals".* **Prof. A. D. Rollett** (from Carnegie Mellon University, Pittsburgh, Pennsylvania, USA). May 2012.

3. *"Polymer nanocomposites with layered minerals – possibilities and limitations".* **Dr. A. Leuteritz** (from Leibniz-Institut für Polymerforschung, Dresden, Germany). August 2012.

4. *"Challenges and opportunities for the development of non-equilibrium phases by the application of pressure and shear".* **Dr. S. Rao Bonta** (from IMDEA Materials Institute, Madrid, Spain). October 2012.

5. *"Carbon Nanotube Fibres: current research and future prospects".* **Prof. A. Windle** (from Cambridge University, UK). October 2012.

6. *"Development of ballistics protections against small fragments for UERF applications".* **F. Martínez-Hergueta** (from IMDEA Materials Institute, Madrid, Spain). November 2012.

7. *"Polymer nanocomposites: preparation techniques and applications".* **Dr. A. Benito** (from Technological Institute of Plastic, AIMPLAS, Valencia, Spain). November 2012.

8. *"Computational thermodynamics/Kinetics and materials genome initiative".* **Prof. Xiao-Gang Lu** (from Shanghai University, China). December 2012.

9. *"Atomistic modelling of silicon recrystallization for advanced nanoelectronics devices".* **B. Sklenard** (from Institute National des Sciences Appliquées, Lyon, France). December 2012.

seminars

6.8. Fellowships

Stage of Professors and Researchers on Sabbatical Year, Spanish Ministry of Education, Culture and Sport

Prof. P. Frontini (University of Mar del Plata, Argentina), July-December 2012

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

Call 2012: **Dr. J. P. Fernández**

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

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

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

Ramón y Cajal Programme, Spanish Ministry of Science and Innovation

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

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

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

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

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

Call 2009: **Dr. A. Jérusalem**

China Scholarship Council

Call 2012: **Y. Chen, X. Zhao**

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

Cajal Blue Brain Project, Spanish Ministry of Science and Innovation

J. García

fellowships

6.9. International Research Internships

Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, (Düsseldorf, Germany).

Research Internship Grant by Max-Planck-Institut, **A. Fernández**

Erich Schmid Institute of Materials Science, Austrian Academy of Science (Leoben, Austria).

Research Internship Grant Ernst-Mach by Austrian Federal Ministry of Science and Research, **E. Moreno**

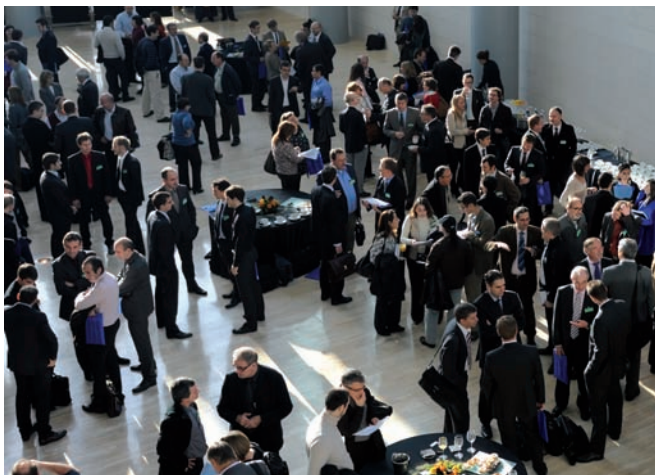
Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing (Michigan, USA)

R. Muñoz

Erich Schmid Institute of Materials Science, Austrian Academy of Science (Leoben, Austria).

Research Internship Grant Ernst-Mach by Austrian Federal Ministry of Science and Research, **R. Soler**

international research internships



awards

6.10. Awards

Fellow, European Mechanics Society (EUROMECH)

Prof. J. LLorca

Shanghai Jiatong University, Shanghai, China, Guest Professorship

Prof. J. LLorca

Young Investigator Award, Polytechnic University of Madrid

Dr. J. Segurado

institutional activities

6.11. Institutional Activities

- Member of the Steering Committee of the *Spanish Technological Platform of Advanced Materials and Nanomaterials* (MATERPLAT)
- Host Institution and co-organizer of the General Assembly of the *Spanish Technological Platform of Advanced Materials and Nanomaterials* (MATERPLAT)
- Host Institution of the EADS International Composite Days
- Member of the Technological Clusters on Security and Renewable Energies promoted by *Madrid Network*.
- Member of the Network of Research Laboratories of *Comunidad de Madrid* (REDLAB)
- Co-organizers of the *Interuniversity Research Seminars Programme* (Dr. C. Dávila, Prof. V. Deshpande)
- Participation in the "*XII Semana de la Ciencia"*, promoted by *Madri+d*
- Participation in the "*Noche de los investigadores",* promoted by *Fundación Madri+d*

6.12. Theses

6.12.1. PhD Theses

"Micromechanical characterisation and simulation of the effect of environmental aging in structural composite materials"
Student: Marcos Rodriguez
Polytechnic University of Madrid
Advisors: Dr. C. González and Dr. J. M. Molina-Aldareguia
Date: February 2012

"High strain rate behavior of Magnesium alloys"
Student: Nathamar Dudamell
Complutense University of Madrid
Advisors: Dr. T. M. Pérez-Prado and Dr. F. Gálvez
Date: December 2012

6.12.2. Master/Bachelor Theses

"Preparation and properties of nanocarbon composites"
Student: Bartomolé Mas
Polytechnic University of Madrid
Advisor: Dr. J. J. Vilatela
Date: March 2012

"Virtual testing of low-velocity impact on CFRP samples"
Student: Koen Valkenhoef
Delft University of Technology
Advisor: Dr. C. S. Lopes
Date: April 2012

"Investigation by means of computed tomography of damage evolution in ±45° carbon fibre laminates"
Student: César Díaz López
Polytechnic University of Madrid
Advisors: Dr. F. Sket and Dr. M. V. Aguirre-Cebrian
Date: July 2012

theses

"Neurite: a finite difference continuum model of the electrophysiological-mechanical coupling in neurons under mechanical loading"
Student: Julián García
Polytechnic University of Madrid
Advisors: Dr. A. Jérusalem and Dr. J. M. Peña
Date: August 2012

"Low strain rate mechanical behavior of Magnesium alloys. Analysis of porosity by X-ray computed assisted tomography"
Student: Daniel Pamplona
Polytechnic University of Madrid
Advisors: Dr. F. Sket, Dr. M. V. Aguirre-Cebrián and N. Dudamell
Date: August 2012

"Bidimensional nucleation on barite surfaces: Observations by atomic force microscopy and Monte Carlo simulations"
Student: Santiago de Antonio Gómez
Complutense University of Madrid
Advisors: Dr. C. Pina and Dr. I. Martín-Bragado
Date: September 2012

"CNT growth on conventional engineering materials"
Student: Máximo García
Carlos III University of Madrid
Advisors: Dr. J. J. Vilatela and Dr. M. E. Rabanal
Date: October 2012

6.13. Internships / Visiting Students

"Microstructural and mechanical characterisation of Fe3Al-based alloys for high temperature applications"
Student: Guang Yang
North China Electric Power University
Advisor: Dr. S. Milenkovic
Date: April-August 2012
Academic Internship Programme for Chinese Technical Students offered by the Polytechnic University of Madrid.

6.14. Courses

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

"Non conventional composites"
Master in Composite Materials
Polytechnic University of Madrid and EADS
Professor: J. J. Vilatela, R. Guzmán, I. Sabirov and J. LLorca

"Structural composite materials"
Master/ Doctoral Program in Engineering of Structures, Foundations and Materials
Polytechnic University of Madrid
Professor: J. LLorca and C. González

"Mechanics of composite materials"
Master/ Doctoral Program in Engineering of Structures, Foundations and Materials
Polytechnic University of Madrid
Professor: J. Segurado and C. González

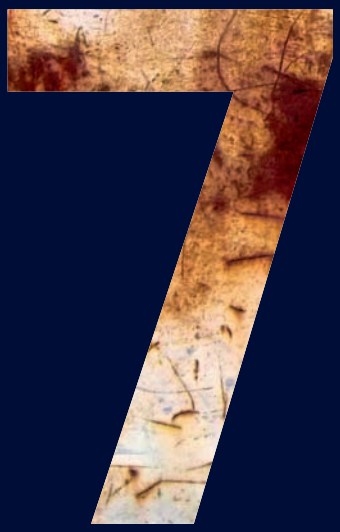
"Advanced powder metallurgy materials"
Master/ Doctoral Program in Materials Science and Engineering, University Carlos III of Madrid
Professor: J. M. Torralba

"Processing of Materials"
Master/ Doctoral Program in Advanced Structural Materials for New Technologies, University Carlos III of Madrid / Rey Juan Carlos University
Professor: J. M. Torralba

courses

internship
visiting students

scientific highlights



annual report 2012

tricking

Tricking nature: Stabilization of metastable metallic phases under ambient conditions

stabilization of metastable metallic phases under ambient conditions

The advent of new materials has been critical to the progress of mankind. Conventional strategies to process advanced metals include alloy design, thermomechanical processing, the fabrication of composites or a combination of all these. However, these methods have limitations. Many alloys present allotropic modifications with unique properties that are stable at extreme temperatures and/or high pressures and which can currently not be exploited. Researchers at IMDEA Materials are devising ways in which these phases can be stabilized at room temperature and atmospheric pressure so that these materials become available for engineering applications.

They have recently succeeded to stabilize ω-Zr, a phase that was so far only stable at pressures higher than about 2 GPa (Fig. 1 [1]), as well as an hcp-Li phase (Fig.2[2]), which had been only found to be stable at temperatures between 70 and 80 K. These metastable phases were obtained by the application of pressure and/or shear at room temperature and have been retained under ambient conditions.

Work in progress includes the extension of this research to other metallic systems, the stabilization of new phases by mechanical milling and consolidation of powders as well as the fabrication of metals with tailored properties by the development of composite multi-phase systems.

nature

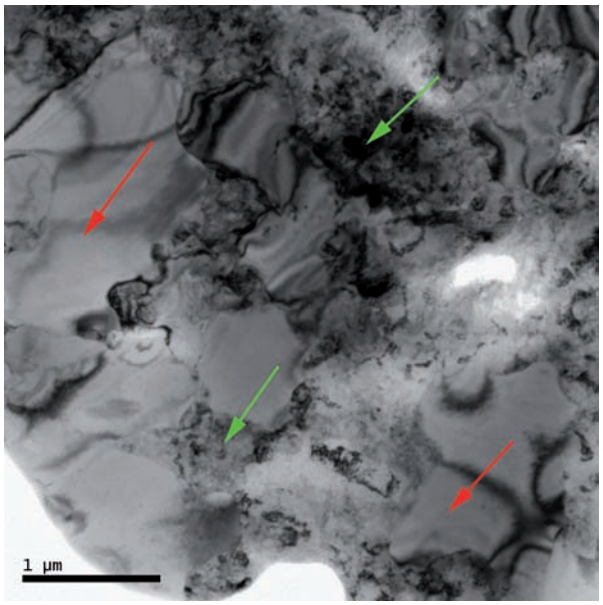


Figure 1. A composite structure formed by α (red arrows) and ω-Zr (green arrows).

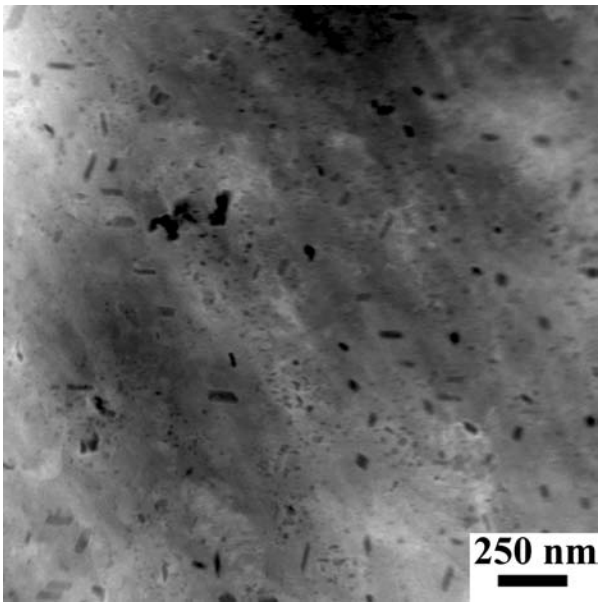


Figure 2. Scanning electron transmission microscopy image illustrating hcp Li particles in a Mg-Li matrix.

References

[1] A. P. Zhilyaev, I. Sabirov, G. González-Doncel, J. M. Molina-Aldareguía, B. Srinivasarao, M. T. Pérez-Prado, Material Science Engineering, 528, 3496-3505, 2011.

[2] B. Srinivasarao, A. P. Zhilyaev, I. Gutiérrez-Urrutia, M. T. Pérez-Prado, Scripta Materalia, 68, 583-586, 2013

synthesis of nan

Synthesis of nano-architectures: the window towards new materials

Chemical Vapor Deposition (CVD) is probably the most versatile technique to produce nano-architectures. Novel nanostructures with extraordinary properties such as vertically aligned carbon nanotubes, ceramic nanorods [1], graphene [2], etc. can be easily synthesized using this approach. One of the main advantages of CVD is its scalability [3], leading to an easy translation from the laboratory to industrial setting.

The Nano-Architectures and Materials Design group at IMDEA Materials Institute has developed an experimental semi-continuous CVD technology especially designed to synthesize vertically aligned nanotubes and graphene. This facility is able to grow nanostructures on substrates of up to 1 m in length and to ramp up the temperature from 30 to 700?C in just 3 minutes.

This unique system provides to IMDEA Materials with a new route to synthesize carbon nanotubes on structural fibres, which are commonly known as fuzzy fibres [4]. These nano-architectures are envisioned to be the next generation of structural fibres for composite materials. Outstanding properties for delamination strength, non-destructive evaluation, de-icing properties, etc. have been demonstrated using these nano-architectures, making the resulting composites truly multifuntional materials [5].

It is also really interesting to synthesize vertically aligned nanotubes on low-cost substrates as metal sheets. Using out-of-the-shelf metal substrates to directly grow CNTs reduces significantly the cost, as this process generally needs silicon wafers processed by expensive micro-fabrication process. These vertically aligned carbon nanotubes can be transferred to other substrates which make this material really interesting for its large surface area and high mechanical strength as well as electrical and thermal conductivity. Because of the potential of these nano-structures, applications in the field of energy storage, actuators, composites, etc. are envisioned.

the window towards new materials

o-architectures

With this unique system, IMDEA Materials Institute is positioned at the forefront of synthesis of nano-architectures for structure, working in one of the most scientifically and technologically exciting fields, as recognized by the European Union and their Flagship program on Graphene, a global project with a budget of 1000 million of euros over the 10 next years.

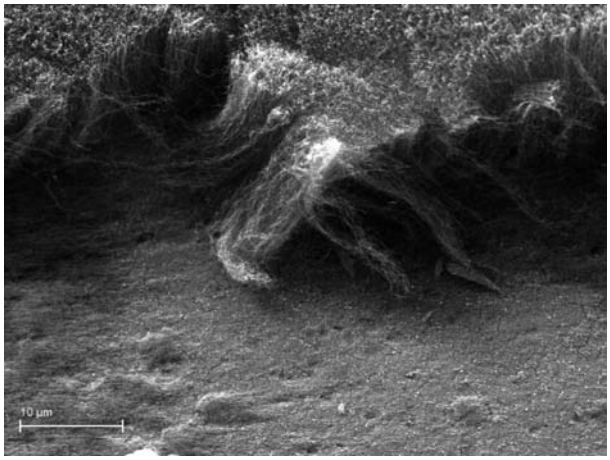


Figure 1. Detail of a vertically aligned carbon nanotubes grown on a low cost metallic foil.

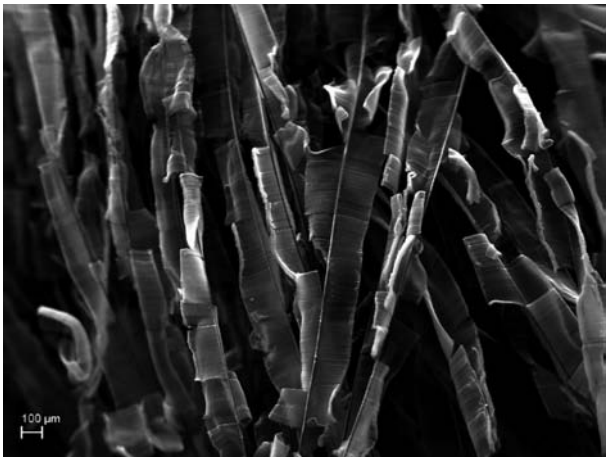


Figure 2. Aligned carbon nanotubes synthesized in the surface of structural fibres. This material is commonly known as fuzzy fibre.

References

[1] C. Klingshirn, "ZnO: Material, Physics and Applications", *ChemPhysChem*, 8, 782–803, 2007.
[2] S. Bae, H. Kim, Y. Lee, X. Xu, J.-S. Park, Y. Zheng, J. Balakrishnan, T. Lei, H. Ri Kim, Y. I. Song, Y.-J. Kim, K. S. Kim, B. Ozyilmaz, J.-H. Ahn, B. H. Hong, and S. Iijima, "Roll-to-roll production of 30-inch graphene films for transparent electrodes", *Nat Nano*, 5, 574–578, 2010.
[3] R. Guzmán de Villoria, A. J. Hart, and B. L. Wardle, "Continuous High-Yield Production of Vertically Aligned Carbon Nanotubes on 2D and 3D Substrates", *ACS Nano*, vol. 5, 4850–4857, 2011.
[4] S. Wicks, R. Guzman de Villoria, and B. L. Wardle, "Interlaminar and Intralaminar Reinforcement of Composite Laminates with Aligned Carbon Nanotubes", *Composite Science and Technology*, 70, 20–28, 2010.
[5] R. Guzman de Villoria, N. Yamamoto, A. Miravete, and B. L. Wardle, "Multi-Physics Damage Sensing in Nano-Engineered Structural Composites", *Nanotechnology*, 185502 (7pp), 2011.

multiscale model

Multiscale modeling of composites: the path to virtual testing and design

the path to virtual testing and design

The presence of different energy dissipation mechanics at various length scales (Fig. 1) calls for a multiscale modelling strategy. Recently, IMDEA Materials developed and validated a coherent multiscale approach to carry out high fidelity simulations of the mechanical performance of composite laminates [1]. As a result, "virtual tests" are starting to be used in engineering applications to limit the number of costly experimental tests to certify safety of composite structures, and the reduction of product development time. Hence, this strategy makes the "virtual design" of laminates affordable, as well as their optimization under non-trivial load cases such as impact loading (Fig. 2).

Multiscale modelling of structural composites has been attempted in the past using the global-to-local approach. Although this strategy has proven very useful from the structural engineering viewpoint, the phenomenological nature of the composite material models limits its ability to extend the results to design optimized lay-up configurations or to carry "virtual tests" of structural components which present very different damage mechanisms upon loading. The new approach developed by IMDEA Materials allows to carry out multiscale modelling by computing the properties of one entity (e.g. individual plies) at the relevant length scale, homogenizing the results into a constitutive model, and passing this information to the simulations at the next length scale to determine the mechanical behaviour of the larger entity (e.g. laminate) [2]. Thus, multiscale modelling is carried out through the transfer of information between the three different length scales rather than by coupling different simulation techniques.

References

[1] J. LLorca, C. González, J .M. Molina-Aldareguía, C. S. Lopes. Multiscale Modeling of Composites: Toward Virtual Testing ... and Beyond. JOM - The Journal of the Minerals, Metals & Materials Society (TMS), 65, 2013.

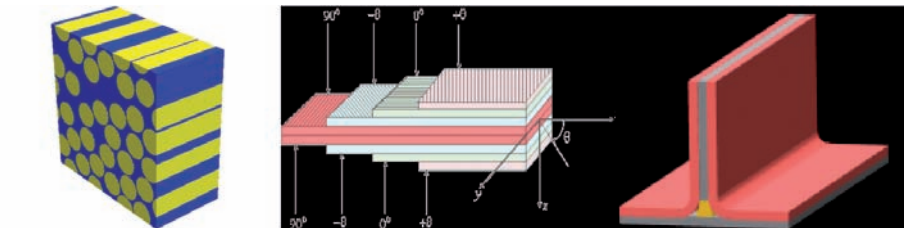
[2] J. LLorca, C. González, J. M. Molina-Aldareguía, J. Segurado, R. Seltzer, F. Sket, M. Rodríguez, S. Sádaba, R. Muñoz, L. P. Canal. Multiscale modeling of composite materials: a roadmap towards virtual testing. *Advanced Materials,* 23, 5130, 2011.

ing of composites

a) ply
fiber diameter: ~10 μm

b) laminate
ply thickness: 150-300 μm

c) component
laminate thickness: 2-20 mm



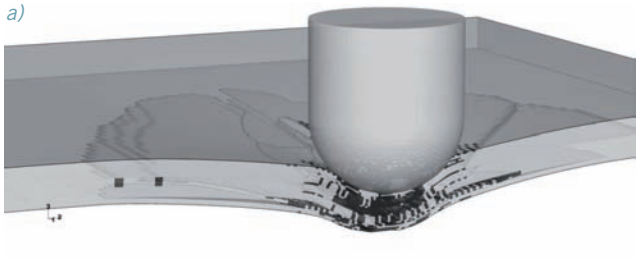
matrix shear yielding
interface decohesion
fiber fracture
fiber kinking

crack bridging
fiber pull-out
matrix cracking
interply decohesion

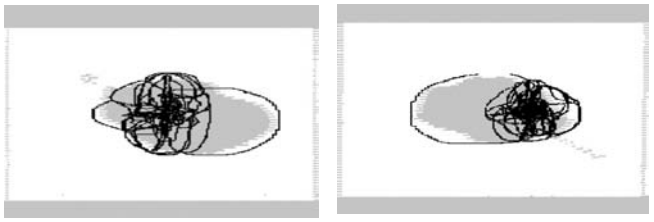
buckling
crushing

Figure 1. Hierarchical structure of composite materials, showing the three entities, their relevant length scale and their dominant energy dissipation mechanisms. (a) Ply. (b) Laminate. (c) Component.

a)



b)



c)

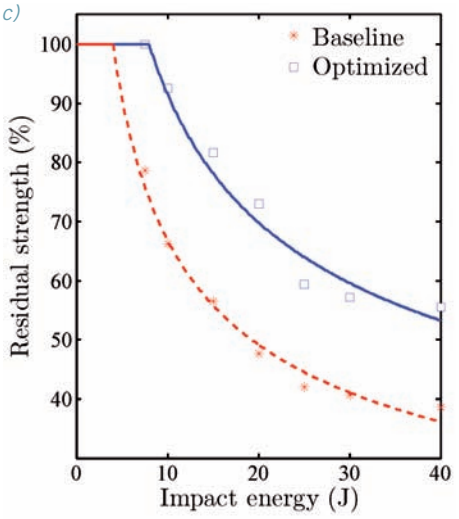


Figure 2. Optimization of composites laminates with virtual testing. (a) Virtual impact test (20J) on a standard coupon showing matrix cracks and delaminations. (b) Impact footprint (superposition of damage at all layers and interfaces) on a traditional laminate (left) and on an optimized configuration (right). The grey areas are the C-scan measurements while the visible dark lines correspond to the numerical prediction of the extent of delaminations at each interface. (c) Normalized residual strength results obtained with compression-after-impact tests.

environment

Environmentally friendly high performance fire retardant polymer nanocomposites

high performance fire retardant polymer nanocomposites

Polymeric materials are now ubiquitous in our day-to-day life in electrical/electronic devices, furniture, transportation, aircraft components, construction, etc. However, flammability is a key limitation in most of them (both natural and synthetic polymers) and their widespread use increases dramatically the fire risk. Fire retardants for polymeric materials are the answer to this problem; however, the increasing use of halogen-based fire retardants in the last decades has had a serious negative impact on the environment due to their toxicity, leading to a strong interest in halogen-free fire retardant materials [1, 2].

The High Performance Polymer Nanocomposites Group has been developing a series of novel environmentally friendly fire retardant polymeric materials by combining molecular design, advanced chemistry synthesis and nanotechnology. A good example of these investigations is the improvement of the fire resistance of polypropylene (PP) through addition of sepiolite based additives (InneoClay 20)*. The flammability and burning behaviour of these new nanocomposites were studied using different experimental techniques such as limiting oxygen index, vertical burning test and cone calorimeter (Figure 1).

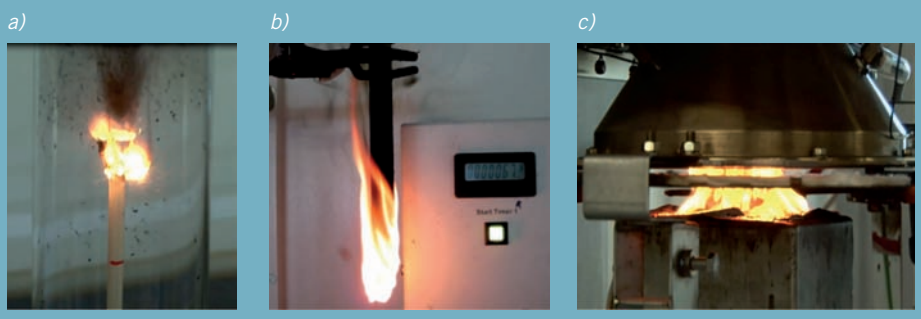


Figure 1. Fire behavior study via (a) limiting oxygen index; (b) vertical burning test; (c) cone calorimeter test.

ally friendly

Compared with traditional fire retardant technology (PP-FR25), the new material with 2% sepiolite-based additive + 23% traditional fire retardant (PP-NFR25) reduces by a factor of ≈3 the maximum heat release rate during burning (Figure 2).

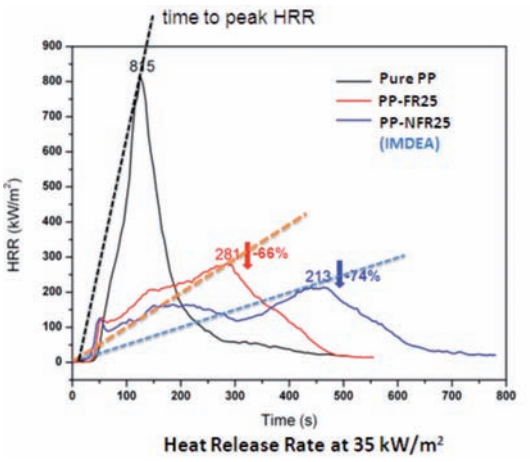


Figure 2. Heat release rate vs time for pure PP, traditional fire retardant (PP-FR25) and novel fire retardant system (PP-NFR25).

In addition, the time necessary to reach the maximum heat release rate was delayed from 285s to 440s in the PP-NFR25 system, leading to a significant improvement in fire safety as compared to the traditional material. This behaviour is due to the formation of a protective char layer on the specimen surface during burning (Figura 3).

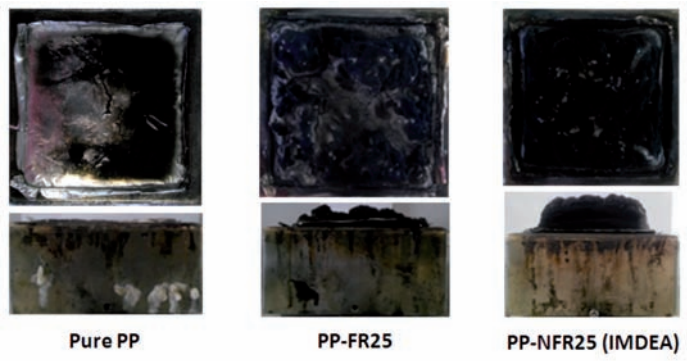


Figure 3. Char residues after burning (via cone calorimeter test at 35 kW/m²) for PP, PP-FR25 and PP-NFR25 composites.

Another important advantage of the new fire retardant materials was the suppression of smoke during burning. As shown in Figure 4, the smoke production of PP-NFR25 decreases over 40 % in comparison to the traditional fire retardant PP-FR25 composite. Furthermore, the smoke release during burning is also delayed.

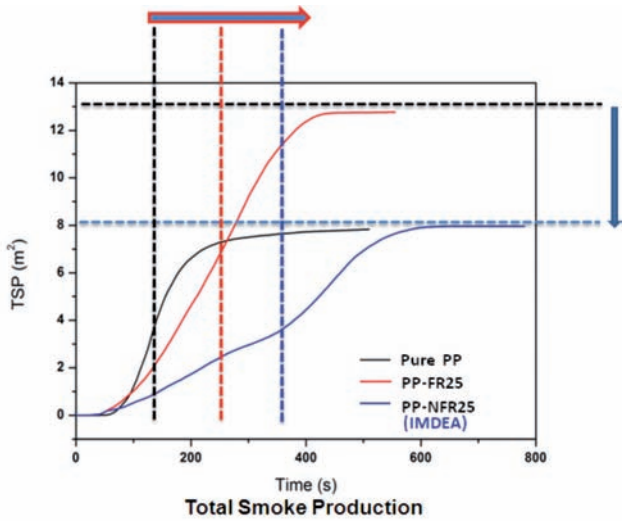


Figure 4. Reduction in total smoke production of new fire retardant (NFR) PP composites as compared to the traditional fire retardant (FR) PP material.

Based on these results, and following the interdisciplinary and innovative approach described above, researchers at IMDEA Materials Institute are working to develop a new generation of eco-benign fire retardant polymers with high added value in different industrial sectors such as electronic/electrical, transportation, construction, etc.

** Samples provided by TOLSA*

References

[1] D.-Y. Wang et al. Synthesis of organo Co–Al layered double hydroxide via a novel single step self-assembling method and its use as flame retardant nanofiller in PP. *Langmuir,* 26, 14162-14169, 2010.

[2] D.-Y. Wang et al. Preparation and burning behaviours of flame retarding biodegradable poly(lactic acid) nanocomposite based on zinc aluminium layered double hydroxide. *Polym. Degrad. Stab.* 95, 2474-2480, 2010.

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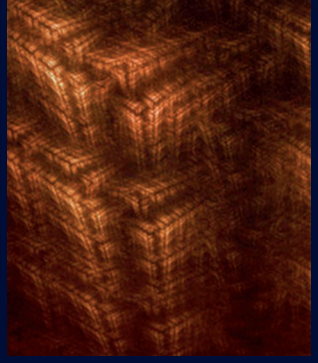

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annual report

2012