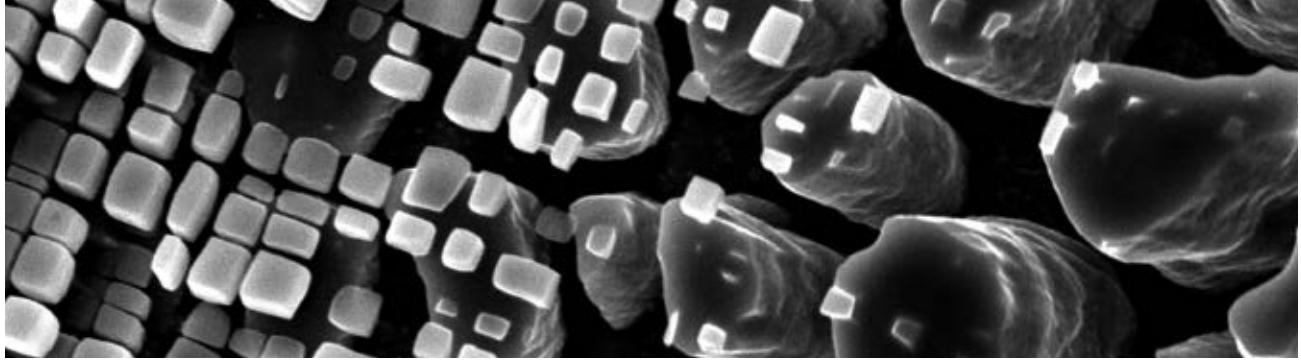

imdea materials institute

excellence as our technological key

institute imdea materials

annual report 2013

foreword

Javier LLorca
Director, IMDEA Materials Institute
March 2014

annual report
2013

2013 has been an international year for IMDEA Materials Institute for various reasons. Firstly, it has been awarded eight new international research projects, including six funded by various instruments of the EU Seventh Framework Programme for Research, one belonging to the Materials World Network, jointly supported by the National Science Foundation of the United States and the Ministry of Economy and Competitiveness of Spain, and one project supported by the Ministry of Science and Education of the Russian Federation. Secondly, four international workshops (devoted to Mg alloys, computational thermodynamics, graphene and 2D materials, as well as nanolaminates) were held at the Institute, taking full advantage of the facilities in the new building. Over 400 researchers from 30 countries attended these events, enhancing the international visibility of our activities. Thirdly, the Institute has attracted more talented individuals from all over the world who come to carry out research excellence in an international and multidisciplinary environment. The current team involves 76 researchers, including eight senior researchers, six researchers, three visiting scholars, 20 post-doctoral researchers and 39 doctoral students, of 13 nationalities, who are supported by an international project management team and six laboratory technicians.

The year has seen new scientific infrastructure installed. They include a chemical vapour deposition reactor to manufacture graphene and other nanomaterials, and a co-rotating twin screw extruder which, together with an injection moulding machine, can be used to process thermoplastic nanocomposites for high-performance applications. In addition, microstructural characterisation capabilities have been greatly improved with the incorporation of a dual beam focused ion beam – field emission gun scanning electron microscope equipped with a detector for secondary, back-scattered and transmitted electrons, X-ray microanalysis and electron backscatter diffraction for 3-D microstructural, chemical and crystallographic orientation analysis. Finally, the high-performance computing cluster has been upgraded to reach three Teraflops.

The research activities in the four research programmes have led to 79 publications in international peer-reviewed journals and three new patent applications, together with 27 plenary/keynote lectures at international conferences and 31 invited seminars at prestigious research institutions and universities throughout the world. All the data show that the IMDEA Materials Institute is rapidly becoming an international player in the competitive research field of materials science and engineering.

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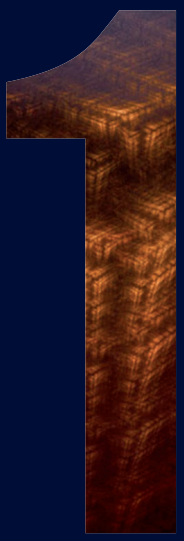
introduction



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1.1 About the IMDEA Materials Institute

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

The 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 Internationalisation strategy

Globalisation is one the key features of the twenty-first century and this is particularly relevant in research. Thus, internationalisation is a strategic activity for IMDEA Materials Institute, which is focussed on the following action lines:

- Attraction of talent from all over the world to Madrid to work in an international and interdisciplinary environment.
- Development of scientific collaboration with universities, research organisations and companies across the world through the participation in research collaborative projects and networks.
- Participation in international R&D programmes with particular emphasis on the EU Framework Programmes for Research (FP7 and H2020).
- Collaboration with both Spanish multinational and foreign companies through R&D contracts to improve their innovation capacity and technological leadership in a global market.
- Consolidation of the international visibility of the Institute within the materials science and engineering scientific community through the organisation of international workshops.

At the beginning of activity in 2007, a strategic plan was designed and implemented to attain these goals. Given the end of the EU Seventh Framework Programme for Research

(2007-2013), 2013 serves as an appropriate moment to summarise the results of the internationalisation strategy, of which the main ones are summarised below:

- 106 researchers from 17 nationalities have worked at the Institute since 2007 of which 47 hold a PhD

- The Institute has participated in 29 European R&D projects funded by the EU sixth and seventh framework programmes for research and coordinated eight of them. The average success rate in the period 2007-2013 (proposals/projects funded) is 32%. In addition, the Institute has participated in other international research programmes supported by the China Scholarship Council (six), the Russian Federation (one) and the Materials World Network (two), jointly funded by the National Science Foundation of the United States and the Spanish Ministry of Economy and Competitiveness.

- The Institute has carried out 25 R&D contracts funded by Spanish multinationals and five funded by foreign companies from Belgium, France, Singapore, the United Kingdom and the United States.

- Four international scientific workshops have been organised in 2013 (see section 6.4), taking advantage of the new facilities inaugurated in 2012.

The start of *Horizon 2020* in 2014 poses a new challenge for the Institute, which is committed to maintaining and increasing the success rate and participation in the programme, with a particular emphasis on the *Excellent Science* pillar. In addition, the internationalisation strategy will also focus on increasing the R&D project portfolio with leading technological firms at both national and international levels.

1.3 Appointments to the Board of Trustees and Scientific Council

- Dr. Rocío Albert López-Ibor, General Director of Universities and Research of the Madrid Regional Government replaced Dr. Jon Juaristi Linacero as one of the permanent trustees from the Regional Government of Madrid.

- Prof. Antonio Hernando, Director of the Institute of Applied Magnetism, Complutense University of Madrid replaced Prof. Juan Manuel Rojo; Dr. Angel Arteaga Iriarte. Director of the Eduardo Torroja Institute for Construction Science (CSIC), replaced Prof. Victor Ramón Velasco; and Prof. Dr. Manuel Laso, professor at the Technical University of Madrid replaced Prof. Manuel Elices, as trustees from universities and public research institutions.

- Dr. Manuel Doblaré, Scientific Director of Abengoa Research S. L. replaced Ms. Francisa Rodríguez, Director of Engineering of Aciturri Aeronáutica S. L., as trustee from privately owned companies.

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

1.4 Organizational chart

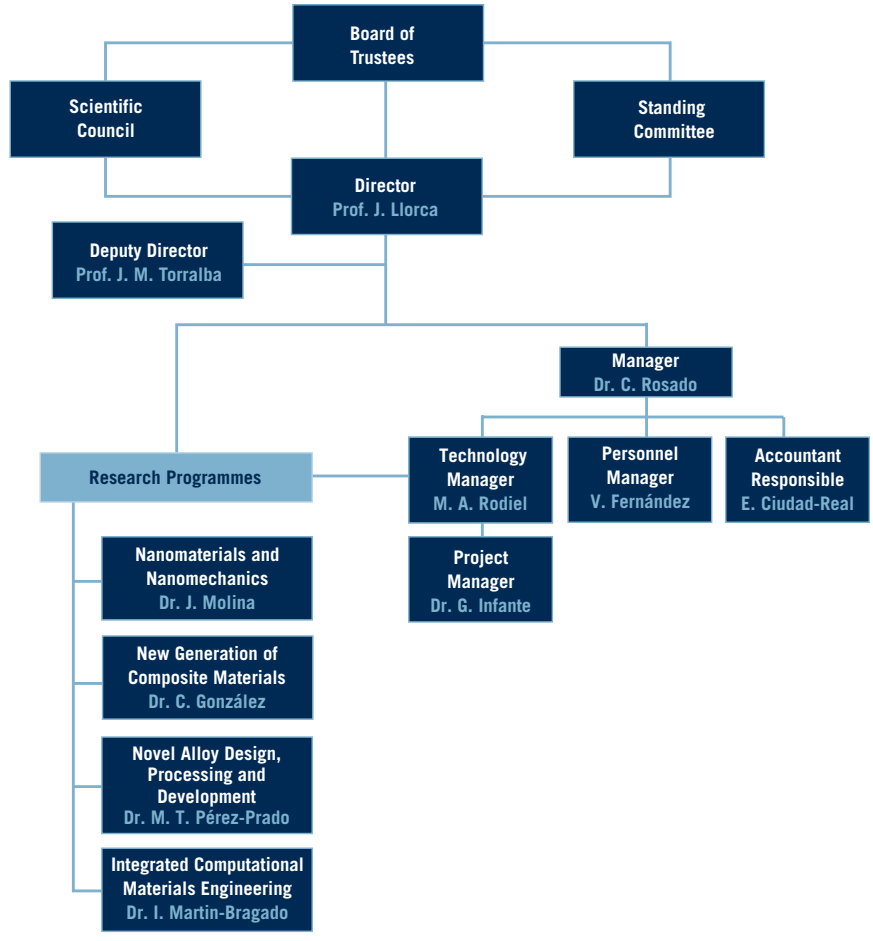


Figure 1. Organizational chart of IMDEA Materials Institute

1.5 Governing bodies

Members of the Board of Trustees

CHAIRMAN OF THE FOUNDATION

Dr. Pedro Muñoz-Esquer
Independent Consultant, Spain

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

Ilma. Sra. Dª Rocío Albert López-Ibor
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)

UNIVERSITIES AND PUBLIC RESEARCH INSTITUTIONS

Prof. Antonio Hernando
Professor
Complutense University of Madrid, Spain

Dr. Angel Arteaga Iriarte
Director
Eduardo Torroja Institute for Construction Science (CSIC), Spain

Prof. Manuel Laso
Professor
Technical University of Madrid, Spain

Prof. Carlos Balaguer
Professor
Carlos III University of Madrid, Spain

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

ABENGOA RESEARCH S.L.
Prof. Dr. Manuel Doblaré
Scientific Director
Seville, 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

Members of the Scientific Council

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

Prof. Brian Cantor
Vice-chancellor
University of Bradford, 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. 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 Institute
Professor, Autonomous University of Madrid, Spain

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

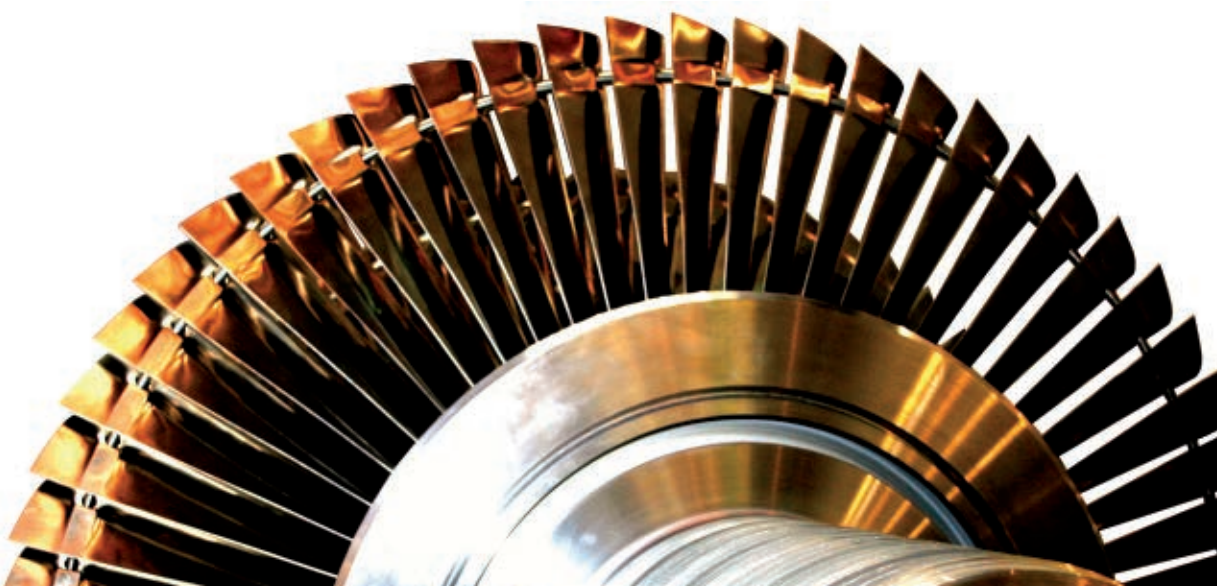
Prof. Pedro Muñoz-Esquer
Independent consultant

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

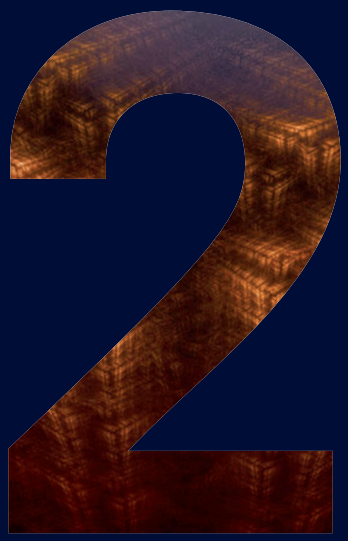
Prof. Gary Savage
Independent consultant

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

These programmes 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.

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.

Driven by the talent of the researchers, research programmes 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 2. Research programmes and strategic partners of IMDEA Materials Institute

Nanomaterials and Nanomechanics

- **Graphene, nanotubes, nanofibers and hybrids:** synthesis, emerging properties and micro / macroscopic applications.
- **Nanomaterials for energy generation and storage:** nanocarbon/semiconductor hybrids for photocatalysis, energy harvesting nanomaterials and capacitors.
- **Hierarchical materials:** materials design from the nanoscale to the macroscale, nano-reinforced materials, composite materials with enhanced electrical and thermal conductivity.
- **Sustainable materials:** bio-based nano-fire retardants, nanocarriers, novel guest-host nanomaterials, nano-cross linkers, functional dye sensitized solar cells, multifunctional polymer nanocomposites, etc.
- **Layer by layer fire retardant nanocoatings**
- **Nanoscale multilayers for extreme environments:** high temperature coatings, radiation resistant multilayers, etc.
- **Size effects in the mechanical behavior of multifunctional materials:** strength of graphene, nanotubes, nanofibers, fibers and their interfaces to exploit their properties in multiscale composite materials. Measuring phase and interphase properties on complex metallic alloys towards microstructural design.
- **High temperature nanomechanics:** high temperature nanoindentation and micropillar compression up to 700 ºC.
- **In situ characterization of materials at the nm and µm scale:** in-situ mechanical testing of composites and metallic alloys (X-ray tomography, scanning electron microscopy).
- **Simulation of the mechanical behavior at the micro and nano-scale:** molecular dynamics, dislocation dynamics, crystal plasticity finite elements.

futurefibres
Tomorrow's innovation

Thomas Swan

INAEL

TOLSA GROUP

ITP
the power of talent

Research groups involved:

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

futurefibres
Tomorrow's innovation

AIRBUS

acciona
Infraestructuras

The Next Generation of Composite Materials

- **Processing of high performance composites:** optimization of out-of-autoclave curing, hot-forming, non-conventional curing strategies, optimization of manufacturing strategies (semicured products).
- **Recycling and repair of structural composites:** green (recyclable) epoxies, electric current-assisted curing for bondings and repairs, effect of ageing on composite performance.
- **New frontiers of structural performance:** high temperature, impact, self-healing, smart materials, self-sensing, non-conventional lay-up configuration, green composites, etc.
- **Composites with multifunctional capabilities:** fire resistance, electrical and thermal conductivity, barrier properties, etc. Hierarchical nanocomposites.
- **Micromechanics of composites:** *in-situ* measurement of matrix, fiber and interface properties, micromechanical-based failure criteria, computational-design of composites with optimized properties (non circular fibers, thin plies, novel fiber architectures, etc.)
- **Virtual testing of composites:** multiscale strategies for design and optimization of composite materials and structures, behavior composite materials and structures under high velocity impact (ice, metallic fragment or blade), crash-worthiness and failure of composite structures, effects of defects.
- **Virtual processing of composites:** multiphysics models of autoclave and out-of-autoclave curing, porosity nucleation and growth during curing.

Research groups involved:

- Structural Composites (Dr. C. González, Programme Leader)
- Design & Simulation of Composite Structures (Dr. C. S. 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)

Novel Alloy Design, Processing and Development

- **Metallic alloys for high temperature structural applications:** Ni/Co-based superalloys for aeroengine components, NiAl intermetallics and TiAl alloys for the next generation of turbine blades.
- **Lightweight (Mg, Al, Ti) alloys and their composites:** development of advanced medical implants from pure Ti and the next generation electrical conductors from Al alloys. Light Mg alloys and nanocomposites for green transport.
- **Physical simulation of metallurgical processes:** development of novel thermo-mechanical processing routes for the fabrication of metallic materials with superior properties; design and optimization of metallurgical processes.
- **High throughput screening of materials:** rapid screening of phases, crystal structures, properties, microstructure and kinetics in bulk materials by the Kinetic Diffusion Multiple Technique; generation of bulk materials libraries for the fast assessment of mechanical properties.
- **Model-based materials design:** integrating molecular dynamics, computational thermodynamics and kinetics, and mesoscale modeling (Landau/Phase Field) of microstructure.
- **Simulation of the mechanical behavior:** development and calibration of microstructural-based constitutive models to predict the mechanical behavior of single crystals and polycrystals. Implementation of the constitutive models in finite element codes to simulate the mechanical behavior.

GRUPO ANTOLIN

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PCB
Precicast Bilbao

MBN nanomaterialia®

Research groups involved:

- Physical Metallurgy (Dr. M. T. Pérez-Prado, Programme Leader)
- 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. Boehlert)

ABENGOA RESEARCH

Integrated Computational Materials Engineering

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GLOBALFOUNDRIES

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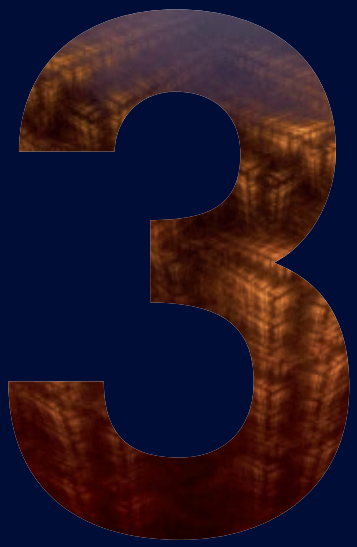
AIRBUS DEFENCE & SPACE

- **Virtual materials design, including virtual processing and virtual testing:** light (Al, Mg and Ti) metallic alloys and their composites, shape memory alloys, Ni-based superalloys, multifunctional composite materials and structures, materials for microelectronics (Si, Ge, InGaAs, etc.) and materials for energy generation and storage.
- **Materials modeling at different length and time scales:** molecular mechanics, molecular dynamics, dislocation dynamics, object and lattice kinetic Monte Carlo, computational thermodynamics and kinetics, microscale-mesoscale-structural scale modeling (Landau/Phase field), numerical methods for solids (finite elements and other approximations for solid mechanics), computational micromechanics, computational mechanics, etc.
- **Multiscale materials modeling:** bottom-up approaches (scale bridging), development of modular multi-scale tools, high throughput screening integration, concurrent models and homogenization theory.

Research groups involved:

- Atomistic Materials Modelling (Dr. I. Martín-Bragado, Programme Leader)
- Mechanics of Materials (Prof. J. LLorca)
- Design and Simulation of Composite Structures (Dr. C. S. Lopes)
- Multiscale Materials Modelling (Dr. J. Segurado)
- Computational Alloy Design (Dr. Y. Cui)
- Computational Solid Mechanics (Prof. I. Romero)

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 currently counts with 76 researchers, including eight senior researchers, six researchers, three visiting researchers, 20 post-doctoral researchers and 39 doctoral students from 13 nationalities. It should be noted that 40% of the researchers are foreign nationals while 57% 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 an international project management team and six laboratory technicians.

senior researchers

Prof. Javier LLorca

Director,
Mechanics of Materials

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

Professor of Materials Science, Technical 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 characterisation 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 Technical 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 Technical University of Madrid. Spain

Associate Professor of Materials Science, Technical University of Madrid

Research Interests

Processing, characterisation 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 (multi-scale models to design novel virtual testing strategies).

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, characterisation 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.

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 characterisation of thin-films, multiphase materials using nanoindentation and advanced focus-ion beam and electron microscopy analysis, mechanical testing inside the scanning electron microscope.

Dr. Javier Segurado

Senior Researcher,
Multiscale Materials Modelling

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

Associate Professor of Materials Science, Technical 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 models. Computational homogenization models and concurrent multiscale techniques for polycrystalline materials. Development of computational micromechanics strategies to simulate the mechanical behaviour until failure of both particle- and fibre-reinforced composites.

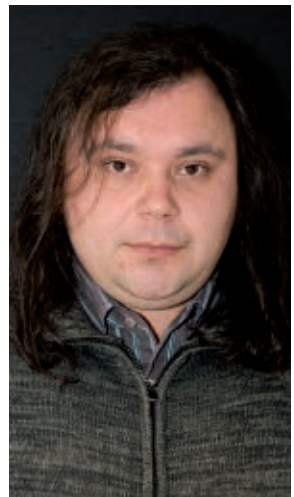
Dr. Ilchat Sabirov

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 that optimise performance of metallic materials.



Dr. De-Yi Wang

Senior Researcher, High Performance Nanocomposites

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

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 nanostructured 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 Science from Central South University. China

Research Interests

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

Dr. 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 characterisation, 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 characterisation 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. TiO_2), 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

Prof. Ignacio Romero

Visiting Scientist,
Computational Solid Mechanics

Ph.D. in Civil and Environmental Engineering from University of California Berkeley USA

Professor. Department of Structural Mechanics and Industrial Constructions. Technical University of Madrid, Spain

Research Interests

Numerical methods for nonlinear mechanics of solids, fluids, and structures. More specifically, development of time integration methods for Hamiltonian and coupled problems, models and numerical methods for nonlinear beams and shells, improvement of finite elements for solid mechanics, error estimators in nonlinear dynamics and multiscale methods for material modelling.

Prof. Mauricio Terrones

Visiting Scientist,
Synthesis and Properties of Novel Nanocarbons

Ph.D. in Chemistry from University of Sussex. UK

Professor of Physics and Materials Science and Engineering, Pennsylvania State University, USA.

Research Interests

Nanostructure synthesis of carbon, graphene and other layered materials, fabrication of nanoscale devices and biocompatible nanocomposites, study of carbon fluidity and metal encapsulated in graphitic sheets, biocompatibility and toxicological effects of doped, functionalized and pure carbon nanotubes and other nanostructures, theoretical studies on novel carbon nanostructures and characterization and microanalysis of nanostructures.

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 Mg structural alloys, and metal matrix composites.

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. Belén Aleman

Postdoctoral Research Associate

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

Research Interests

Growth and doping of semiconductor micro- and nanostructures, characterization of semiconductor micro- and nanostructures by cathodoluminescence within the scanning electron microscope and micro-photoluminescence by optical and confocal microscopy, analysis of chemical composition and structure by energy-dispersive X-ray microanalysis and Raman confocal microscopy, XPS spectroscopy and microscopy in ultra-high vacuum systems under synchrotron radiation.

Dr. Carmen Cepeda

Postdoctoral Research Associate

Ph.D. in Chemistry from University of Alicante. Spain

Research Interests

Study of the relationship between microstructure and mechanical properties of advanced metallic alloys, thermo-mechanical processes based on severe plastic deformation, processing and characterization of multilayer materials with high damage tolerance based on high-strength aluminium alloys for aerospace applications.

Dr. Hyung-Jun Chang

Postdoctoral Research Associate

Ph.D. in Materials Engineering from Grenoble INP, France and Seoul National University, South Korea

Research Interests

Multiscale materials modelling (molecular dynamics, dislocation dynamics, crystal plasticity and finite elements) and fundamental theories (crystal plasticity, dislocation dynamics, size effects and texture) with applications to macroscale (fracture, hydroforming, equal channel angular pressing, drawing and friction stir welding) and nanoscale (void growth and nanoindentation).

Dr. Manuela Cano
Postdoctoral Research Associate

Ph.D. in Materials Science from University of Zaragoza. Spain

Research Interests
Nano-architectures based on carbon materials such as carbon nanotubes and graphene, synthesis from atomic scale of smart materials with enhanced mechanical, thermal and/or electrical properties.

Dr. Aitor Cruzado
Postdoctoral Research Associate

Ph.D. in Industrial Engineering from Mondragon University. Spain

Research Interests
Fatigue and fracture modelling, multiscale modelling (crystal plasticity and finite element method), modelling of fretting and wear, structural integrity.

Dr. Juan Pedro Fernández
Postdoctoral Research Associate

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

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

Dr. Bin Gan
Postdoctoral Research Associate

Ph.D. in Materials Science and Engineering from Illinois Institute of Technology. USA

Research Interests
Superalloys, intermetallics, structural materials, semiconductors, thin films and hard coatings; high temperature nanomechanics and micromechanics; grain boundary engineering and electron backscatter diffraction techniques.

Dr. Andrea García-Junceda
Postdoctoral Research Associate

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

Research Interests
Materials characterization, optimization of the mechanical properties of metallic alloys by modification of their processing route, study and optimization of novel structural materials for energy generation plants, fabrication of oxide-dispersion strengthened alloys by powder metallurgy and optimization of their properties.

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 characterisation by means of optical / electron microscopy and texture analysis.

Dr. Nianjun Kang
Postdoctoral Research Associate

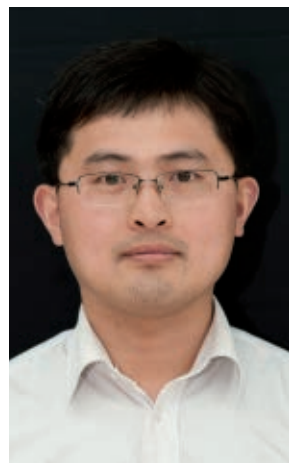
Ph.D. in Materials Science and Engineering from Beijing University of Chemical Technology. China

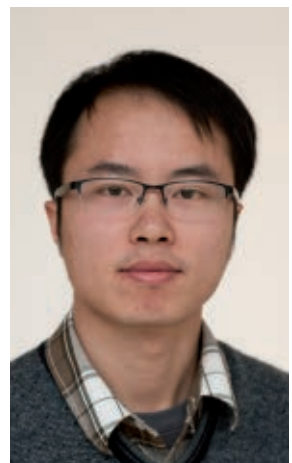
Research Interests
Design, synthesis and characterization of environmentally friendly fire retardant materials, multifunctional materials and polymer nanocomposites.

Dr. Bin Tang
Postdoctoral Research Associate

Ph.D. in Materials Science from Northwestern Polytechnical University. China.

Research Interests
Phase field modelling of phase transformation in metals, solid phase transformation and relationship between microstructure evolution and mechanical properties in high strength Ti alloys, thermal deformation and solid-state diffusion bonding of γ-TiAl alloys, finite element simulation of plastic deformation for structural design.





Dr. Dong-Wook Lee
Postdoctoral Research Associate

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

Research Interests
Phase field modelling of solid-state phase transformation, mesoscale modelling of dislocations and fracture.

Dr. Miguel Monclús
Postdoctoral Research Associate

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

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

Dr. Diego Fernando Mora
Postdoctoral Research Associate

Ph.D. in Structural analysis from Technical University of Cataluña. Spain

Research Interests
Structural analysis on problems of the continuum mechanics by means of numerical methods, structural analysis of composite materials, seismic and dynamic engineering, constitutive equations for new materials, computational mechanics of materials, fracture mechanics of composite materials, simulation of control systems to structures (applications to civil structures).

Dr. Srinivasa Rao Bonta
Postdoctoral Research Associate

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

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

Dr. Federico Sket
Postdoctoral Research Associate

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

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

Dr. Guillermo Vigueras
Postdoctoral Research Associate

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

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

Dr. Jintao Wan
Postdoctoral Research Associate

Ph.D. in Chemical Engineering from Zhejiang University. China.

Research Interests
Thermal analysis of polymer materials, environmentally friendly thermosetting polymers from renewable feedbacks, polymer reaction engineering and polymer product engineering, high performance, flame retardant and low smoke polymer composites.

Dr. Xin Wang
Postdoctoral Research Associate

Ph.D. in Safety Science and Engineering from University of Science and Technology of China. China.

Research Interests
Flame retardant polymer-based nanocomposites, synthesis of halogen-free flame retardants, UV-curing flame retardant coatings.

research assistants

Laura Agudo

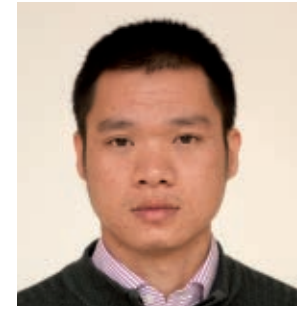
MEng: Rey Juan Carlos University. Spain
Research: Multiscale materials modelling

Marta Cartón

MSc: Carlos III University of Madrid. Spain
Research: Co-based superalloys for high temperature applications

Yi Chen

MEng: Northwestern Polytechnical University. China
Research: Thermo-kinetic study of near beta Ti alloys



Wenzhou Chen

MSc: Northwest University. China
Research: DFT/MD calculation of phase change materials

María Irene de Diego

MEn.: Carlos III University. Spain
Research: Advanced high strength steels

Ignacio Dopico

MEng: Autonomous University of Madrid-CIEMAT. Spain
Research: Atomistic materials modelling

Ana Fernández

MEng: Carlos III University of Madrid. Spain
Research: Crystal plasticity modelling

Julián García

M.Eng.: Technical University of Madrid. Spain
Research: Biological cell modelling

Alejandro García

MEng: Carlos III University of Madrid. Spain
Research: High energy impact on aeronautical composite structures

José Luis Gómez-Sellés

MEng: Complutense University of Madrid. Spain
Research: Atomistic materials modelling

Silvia Hernández

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

Miguel Herráez

MEng: Carlos III University of Madrid. Spain
Research: Nano-architectures and materials design

Luis Carlos Herrera Ramírez

MEng: Carlos III University of Madrid. Spain
Research: Impact in composite materials

Mohammad Ali Jabbari

MEng: Isfahan University of Technology. Iran
Research: Solid state processing of metallic alloys

Ehsan Naderi Kalali

MEng: Pune University. India
Research: High-performance polymer nanocomposites

Yang Lingwei

MEng: Central South University. China
Research: Nanoscale metal-ceramic multilayers

Saeid Lotfian

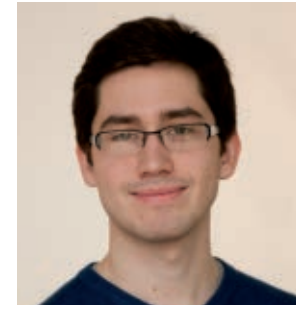
MEng: Isfahan University of Technology. Iran
Research: High temperature nanoindentation

Francisca Martínez

MEng: Carlos III University of Madrid. Spain
Research: Numerical simulation of composites under Impact

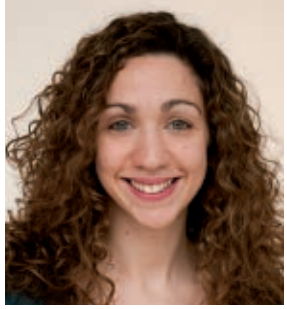
Bartolomé Mas

MEng: Technical University of Madrid. Spain
Research: Multifunctional composites based on CNT fibres



Alfonso Monreal

MEng: Technical University of Madrid. Spain
Research: Production and properties of thermoset nanocomposites



Eva Cristina Moreno

MEng: University of Castilla la Mancha. Spain
Research: Mechanical Behaviour of nanostructured metals

Alicia Moya

MSc: Complutense University of Madrid. Spain
Research: Nanohybrids for photocatalysis

Rocio Muñoz

MSc: Complutense University of Madrid. Spain
Research: Ti-Al intermetallic alloys

Raul Muñoz

MEng: Carlos III University of Madrid. Spain
Research: Computational mechanics of composite materials

Fernando Naya

MEng: Polytechnic University of Madrid. Spain
Research: Multiscale simulation of composites

Alberto Jesús Palomares

MEng: University of Extremadura, Spain
Research: Micromechanics of intermetallic materials

Yetang Pan

MSc: Harbin Institute of Technology. China
Research: Fire retardant polymeric materials

Mónica Prieto

MEng: Technical University of Madrid. Spain
Research: Computer simulation of dislocations

Mehdi Rahimian

MEng: Malek Ashtar University of Technology. Iran
Research: Solidification of Ni-based superalloys

Daniel Rodriguez

MEng: Technical University of Madrid. Spain
Research: Multiscale plasticity

Pablo Romero

MEng: Technical University of Madrid. Spain
Research: Nano-architectures and materials design

Sergio Sádaba

MEng: Public University of Navarre. Spain
Research: Virtual testing of composites

Raúl Sánchez

MEng: University of Cantabria. Spain
Research: Nanoindentation of light alloys

Rafael Soler

MEng: Cranfield University. UK
Research: Nanomechanics

Arcadio Varona

MEng: 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

MEng: Central South University. China
Research: Computational alloy design

Hangbo Yue

MEng: Zhongkai University of Agriculture and Engineering. China
Research: Ecofriendly polymer nanocomposites

Xiaomin Zhao

MEng: Shanghai Jiao Tong University. China
Research: Polymer nanocomposites

laboratory technicians

Marcos Angulo

V.T.: Specialist Technician. Spain

Miguel de la Cruz

V.T.: Specialist Technician. Spain

José Luis Jiménez

V.T.: Specialist Technician. Spain

Vanesa Martínez

MEng: University of Valencia. Spain

Victor Reguero

MEng: University of Valladolid. Spain

Juan Carlos Rubalcaba

BEng: Alcalá de Henares University. Spain

general management

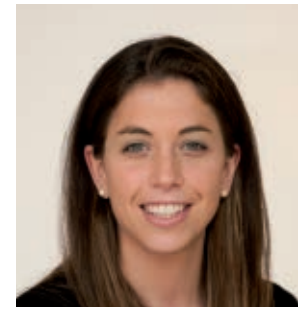
Dr. Covadonga Rosado
Manager

Vanessa Fernández
Personnel Manager

Eduardo Ciudad-Real
Accountant Responsible

Elena Bueno
Executive Secretary

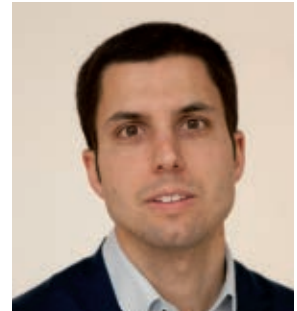
Mariana Huerta
Administrative Assistant



international project office

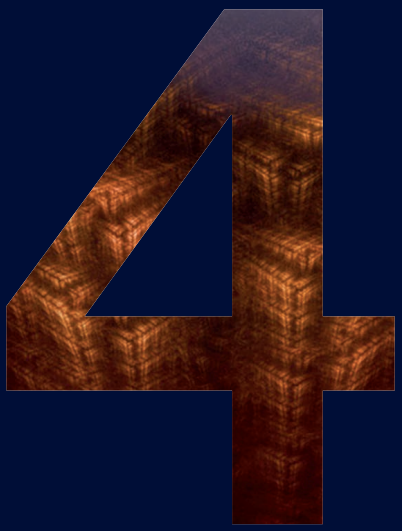
Miguel Ángel Rodiel
Technology Manager &
Project Office Responsible

Dr. Germán Infante
R&D Project Manager



Borja Casilda
Administrative Assistant

research infrastructure



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4.1 Processing

- **Injection Moulding Machine (2013 new equipment)** (Arburg 320 C) to carry out high pressure injection of the raw material into a mould which shapes the polymer into the desired shape. Injection moulding can be performed with commonly thermoplastic polymers and is widely used for manufacturing a variety of parts.

- **Extruder (2013 new equipment)** (KETSE 20/40 EC, Brabender) co-rotating twin screw extruder which offers a variety of thermoplastic polymers processing possibilities. It has an integrated drive with a power of 11 kW and reaches speed up to max. 1200 rpm. Output is in the range of 0.5 - 9 kg/h.

- **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 Vapour Deposition 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 (T_{max}=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 mm) 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.

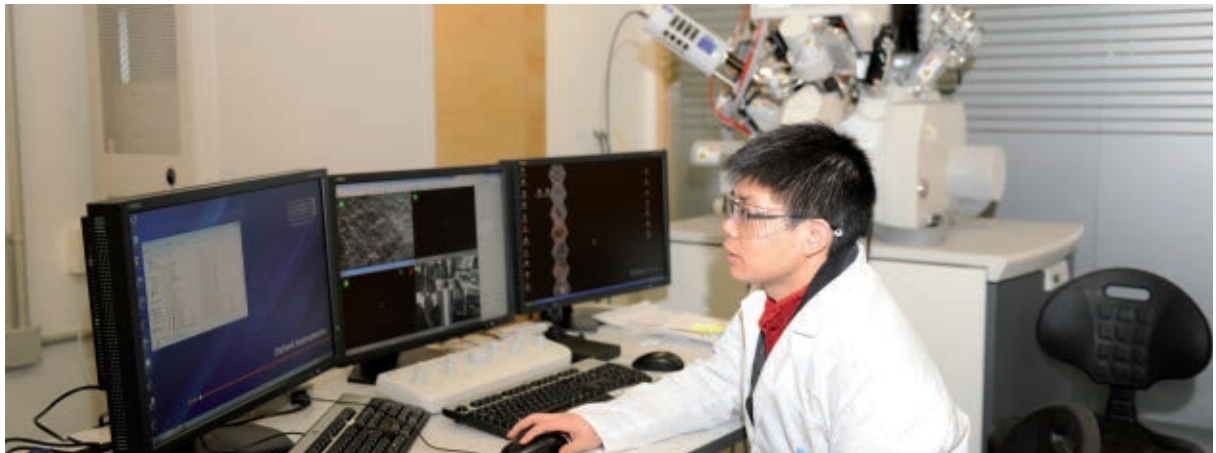
- **Electrospinning Unit** (NANON-01A, MECC) to produce non-woven nanofibrous mats as well as aligned bundles of nanofibres based on various polymers, ceramics and composites. Nanofibres of different shape (smooth and porous surfaces, beaded, core-sheath) and orientations (non-woven cloth, aligned, and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

4.2 Microstructural Characterisation

- **FIB-FEGSEM dual-beam microscope (2013 new equipment)** (Helios NanoLab 600i, FEI) fully equipped with STEM detector, X-Ray microanalysis (EDS) and electron backscatter diffraction (EBSD) for 3-D microstructural, chemical and crystallographic orientation analysis. The system is also suited for site-specific TEM sample preparation, micro machining and patterning by ion-beam milling.

- **FTIR spectrometer (2013 new equipment)** (Nicolet iS50) to measure infrared spectra of absorption, emission, photoconductivity or Raman scattering of a solid, liquid or gas from far-infrared to visible light. It is equipped with the smart accessories of ATR, temperature-dependence and TGA interface.



- **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.

- **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 characterisation 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.

- **Sample Preparation Laboratory** furnished with the following equipment: i) two cutting machines that allow for both precision slicing as well as cutting of large sample, ii) a wire cutting saw, iii) three polishing wheels (one manual, two automatic), including one for the preparation or large, planar sample, and iv) two electrolytic polishing machines, one for double-sided samples, suitable for TEM disk finishing, and one for one-side surface finishing of bulk samples..

- **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 is **regular user of the National Centre for Electron Microscopy**, with **access to several Transmission Electron Microscopes** and facilities for TEM sample preparation. They include several FEG-TEM analytical instruments equipped with X-Ray Microanalysis, EELS, STEM and HAADF, as well as a new aberration-corrected TEM.

4.3 Mechanical Characterisation

- **High Temperature Nanoindentation system (Nanotest Vantage, Micro Materials)** to perform instrumented nanoindentation at temperatures up to 750°C in air and 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 extensome

- **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 Characterisation

- **Thermal conductivity analyser** (TPS 2500 S Hot Disk) to measure the 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 (HRR), peak of HRR, mass loss rates, smoke production, CO_2 and CO yields, effective heat of combustion, and specific extinction areas are directly measured according to ASTM/ISO standards.

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

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

- **Differential Scanning Calorimeter** (Q200, TA Instruments) to analyse 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 cooling system to operate over a temperature range of –40ºC to 400ºC and high cooling rates of ~50ºC/min.

- **Thermogravimetric Analyser** (Q50, TA Instruments) to understand the thermal stability and composition up to 1000ºC by analysing the weight changes in a material as a function of temperature (or time) in a controlled atmosphere.

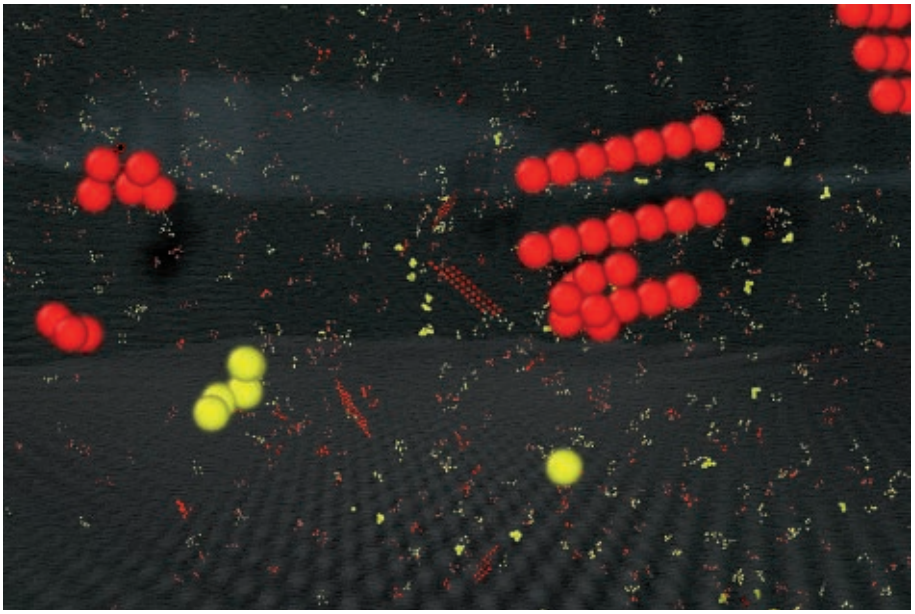
- **High Temperature Furnace** (Nabertherm, RHTH 120/600/16) to carry out heat treatments up to 1600ºC in vacuum or inert atmosphere.

4.5 Simulation

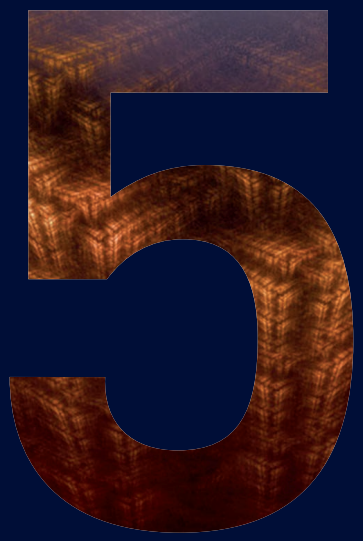
- **High performance computing cluster (upgraded in 2013)** made up of 400 cores Intel Xeon & AMD Opteron with a computing power of 3 Tflops.
- Access to CeSViMa (Madrid Centre for Supercomputing and Visualization) and Mare Nostrum (Barcelona Supercomputing Centre) supercomputing facilities.
- Standard simulation, preprocessing and postprocessing programs (CALPHAD, DICTRA, Micress, Abaqus, LS-Dyna, 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.

4.6 Machine Workshop

The research efforts of IMDEA Materials Institute are supported by the machine workshop which is equipped with a range of machine tools including: conventional lathe (S90VS-225, Pinacho), column drilling machine (ERLO TSAR-35) with automatic feed, surface grinding machine (SAIM Mod. 520 2H) with an electromagnetic table and automatic feed, vertical band-saw table (EVEI SE-400) with electronic speed variator, manual belt-saw (MG CY-270M) for iron and steel cut from 0º to 60º, heavy duty downdraft bench (AirBench FP126784X) and turret milling machine (LAGUN FTV-1).



current research projects



annual report

2013

The IMDEA Materials Institute currently participates in 47 research projects, 16 of which began in 2013. Project funding coming from European projects and industrial contracts increased by 32% and 8%, respectively, year on year. The project portfolio is divided into three main groups: 26 projects were obtained in international competitive calls, out of which 18 are funded by the European Union, five by the Chinese Scholarship Council, two jointly supported by the National Science Foundation of the United States and the Spanish Ministry of Economy and Competitiveness (MINECO) within the Materials World Network Programme, and one funded by the Russian Federation. Six projects are supported by research programmes 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 Industrial Technological Development (CDTI).

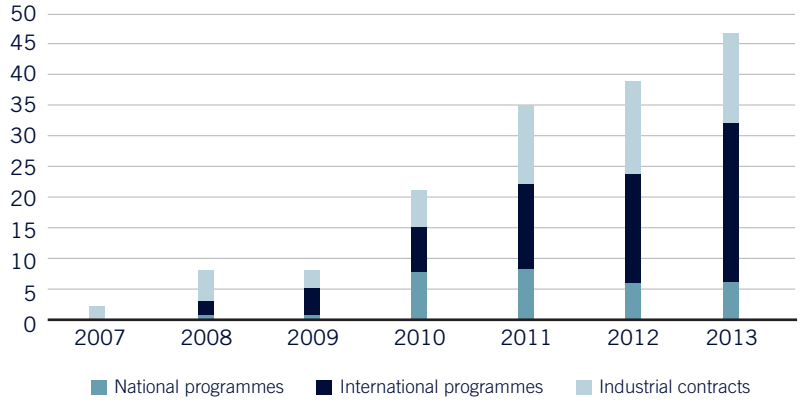


Figure 3. Number of active research projects by funding source

A brief description of the projects which started in 2013 is provided below:

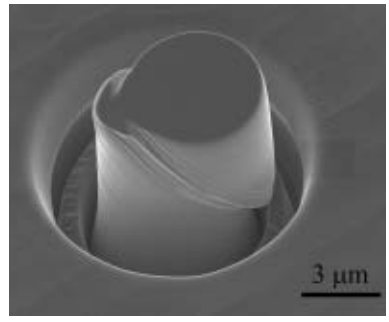
MICROMECH

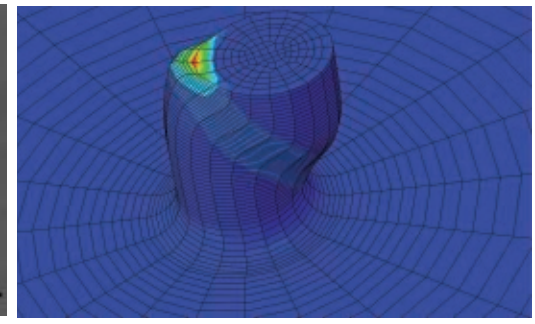
"Microstructure based material mechanical models for superalloys"

Funding: **Clean Sky Joint Undertaking, EU Seventh Framework Programme for Research (FP7)**
Partners: IMDEA Materials Institute
Duration: **2013-2015**
Principal Investigator: **Dr. J. Segurado**

This ambitious two-year research project aims to develop a material model to simulate the mechanical behaviour of polycrystalline Ni-based superalloys processed by casting and forging.

The model will be based on a multiscale approach in which deformation and failure mechanisms as well as microstructural features and defectology, are progressively incorporated at three levels: micron-sized single crystals and small size polycrystals, polycrystalline specimens and components. In such a way, the microstructural features which control mechanical performance (precipitate structure, grain size, texture, porosity and surface condition, among others) can be considered at the appropriate length scale. The proposed model will address the effect of temperature (from room temperature up to 700ºC) in the mechanical properties used in the design of aircraft turbine components: tensile strength, fatigue, crack propagation and creep. In addition, statistical aspects associated with the scale up from polycrystalline specimens to actual components will be incorporated.





SEVENTH FRAMEWORK PROGRAMME

CARINHYPH

"Bottom-up Fabrication of Nanocarbon-Inorganic Hybrid Materials for Photocatalytic Hydrogen Production"

Funding: **NMP, EU Seventh Framework Programme for Research (FP7)**
Partners: IMDEA Materials Institute (Coordinator, Spain), Westfälische Wilhelms Universität Münster (Germany), Thomas Swan & Co (United Kingdom), University of Cambridge (United Kingdom), Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany), Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali, INSTM (Italy), INAEL Electrical Systems (Spain) and EMPA (Switzerland)
Duration: **2013-2015**
Principal Investigator: **Dr. J. J. Vilatela**

This collaborative project, coordinated by the IMDEA Materials Institute, gathers a group of European researchers and industrialists to produce new hybrid nanomaterials for more efficient hydrogen production through photocatalytic water splitting. The aim of the project is to produce materials with superior photocatalytic efficiency by combining nanocarbons (carbon nanoTubes and graphene) with photoactive nanoinorganics such

as metal oxides. Besides hydrogen production (the main project goal), these hybrids also offer significant potential in other applications, such as solar energy conversion by dye-sensitised solar cells, that is to say, "Grätzel cell", water and air purification, self-cleaning surfaces, supercapacitors, and batteries, among others.

Besides the overall technical and management coordination of the consortia, the main contributions offered to the project by the Institute are: purification, functionalisation and characterisation of building blocks, production of hybrids by electrospinning and using pre-assembled nanocarbon architectures, and characterisation of hybrids and interfacial processes.

PilotManu

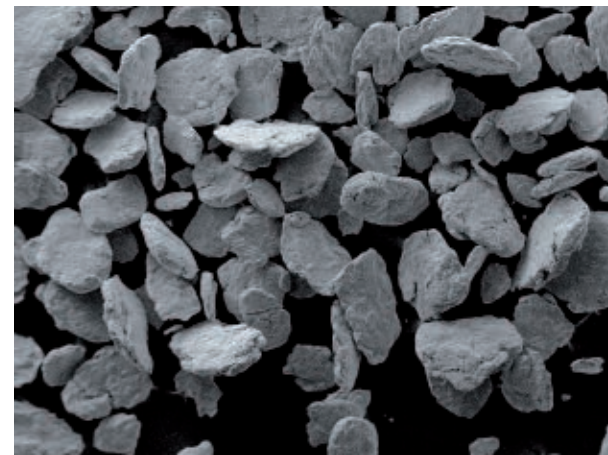
"Pilot manufacturing line for production of highly innovative materials"

SEVENTH FRAMEWORK PROGRAMME

Funding: **NMP, EU Seventh Framework Programme for Research (FP7)**
Partners: MBN Nanomaterialia (Coordinator, Italy), IMDEA Materials Institute (Spain), +90 (Turkey), Putzier (Germany), INOP (Poland), Manudirect (Italy), Centre for Process Innovation (United Kingdom), IMPACT INNOVATIONS GmbH (Germany), Matres (Italy) and Diam Edil SA (Switzerland)
Duration: **2013-2017**
Principal Investigator: **Prof. J. M. Torralba**

The objective of PilotManu is to lower the barriers to market entry for the use of highly innovative advanced materials by scaling up the current research-scale mechanical alloying facility into a powder manufacturing industrial pilot line. This will increase productivity of the technology, enabling supply of cost-effective and high-quality materials which will then be evaluated in several commercial applications. The project will demonstrate the technological and economic viability of the pilot line by incorporating these advanced materials into coatings, abrasive tools and additive manufacturing applications.

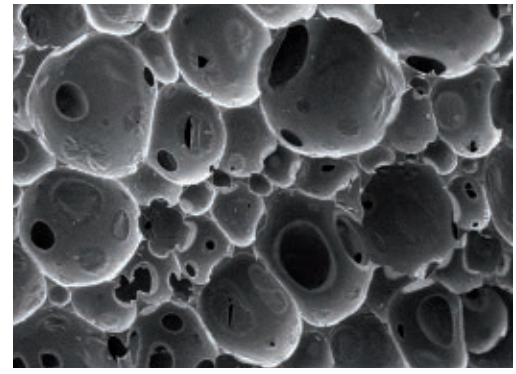
In PilotManu, the IMDEA Materials Institute will focus on the development of bulk materials through field-assisted hot pressing and in the characterisation of the developed materials and products.



SEFIRE

"Study of sepiolite-based fire retardant systems"

Funding: **TOLSA S.A. (Spain)**
Duration: **2013-2014**
Principal Investigator: **Dr. D-Y Wang**



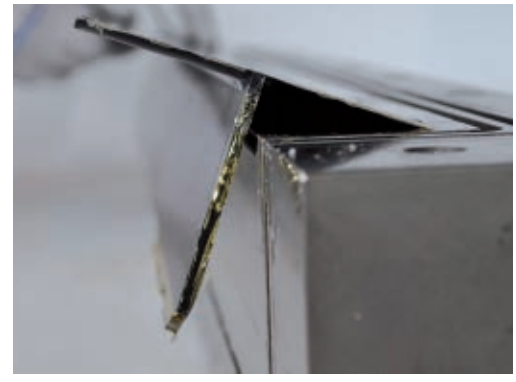
This research contract funded by TOLSA S.A. seeks to study the performance of sepiolite-based additives in fire retardant systems.

In the SEFIRE project, the effect of sepiolite-based additives on fire retardancy of commercial polymer systems is determined by cone calorimeter test. The investigation will also include study of fire behaviour, fire retardant mechanisms, mechanical properties, thermal stability and structure of the char after burning.

SEMICURED STRINGERS

"Highly Integrated semi-cured parts"

Funding: **Airbus Operations S.L. (Spain)**
Duration: **2013-2014**
Principal Investigator: **Dr. C. González**

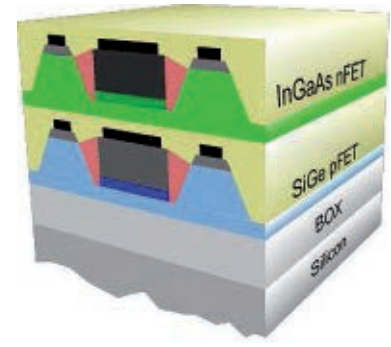


This research contract funded by Airbus Operations S.L. is based on previous experience of IMDEA Materials Institute in the field of semicured panels manufacturing. A new mould for a stringer manufactured by resin-transfer moulding is being designed to achieve a targeted degree of cure, as well as the required dimensional tolerance. In addition, a detailed study of the processing conditions and the final mechanical properties is being carried out to address stringer integration into a component.

COMPOSE3

"Compound Semiconductors for 3D integration"

Funding: **ICT, EU Seventh Framework Programme for Research (FP7)**
Partners: IBM Research GmbH (Coordinator, Switzerland), STMicroelectronics-Crolles (France), Commissariat à l'Energie Atomique-Leti (France), University of Glasgow (United Kingdom), Tyndall National Institute (Ireland), Centre National de la Recherche Scientifique (France), DTF Technology GmbH (Germany) and the IMDEA Materials Institute (Spain)
Duration: **2013-2016**
Principal Investigator: **Dr. I. Martín-Bragado**



This collaborative research project, coordinated by IBM Research in Zurich, focuses on an alternative approach to extend Moore's Law. The new strategy devised in the COMPOSE3 project is based both on use of new materials to replace today's silicon and on an innovative device design, where transistors are stacked vertically, known as 3D stacking. The objective is a 3D stacked SRAM cell, designed with a gate length taken from the 14 nm technology node. This technology will provide a new paradigm shift in density scaling combined with a dramatic increase in the power efficiency of complementary metal-oxide-semiconductor (CMOS) circuits.

The IMDEA Materials Institute will use a lattice kinetic Monte Carlo approach to simulate the physical mechanisms of source/drain regrowth modelling in III-V and IV materials for hybrid microelectronic devices. The models will include a crystallographic and chemical component to account for the structure coupled with a stress analysis by the finite element in the regrown layers. The aim is to create models to optimise source/drain regrowth and advance the current understanding of such a process.

ECURE

"Electrically-curable resin for bonding/repair"

Funding: **Airbus Operations S.L. (Spain)**
Duration: **2013-2014**
Principal Investigator: **Dr. J. J. Vilatela**

ECURE is research contract funded by Airbus Operations S.L. to develop thermoset resins/adhesives that can be cured by directly passing electric current through them. The main idea of the project is to assess the viability of a new out-of-autoclave efficient curing method with high potential for composite bonding and repair.

NONCIRC

"Non-circular carbon fibres"

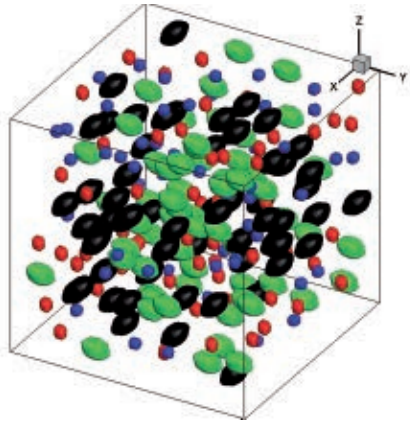
Funding: **Airbus Operations S.L. (Spain)**
Duration: **2013-2014**
Principal Investigator: **Dr. R. Guzmán de Villoria**

NONCIRC is research contract funded by Airbus Operations S.L. to explore the potential of a new kind of non-circular continuous carbon fibre for composites. It is expected that non-circular fibres will provide better longitudinal and transverse mechanical properties to improve the intra-laminar and inter-laminar behaviour of the composite structures, leading to weight reductions.

ICMEG

"Integrative Computational Materials Engineering Expert Group"

Funding: **NMP, EU Seventh Framework Programme for Research (FP7)**
Partners: ACCESS e.V. (Germany), K&S GmbH Projecktmanagement (Germany), e-Xtream engineering S.A. (Belgium), IMDEA Materials Institute (Spain), Thermo-Cal Software AB (Sweden), Stichting Materials Innovation Institute (Netherlands), Czech Technical University in Prague (Czech Republic), RWTH Aachen Technical University (Germany), Centre for Numerical Methods in Engineering (Spain), simufact engineering GmbH (Germany) and Kungliga Tekniska Högskolan (Sweden)
Duration: **2013-2016**
Principal Investigator: **Dr. Y. Cui**



The Integrated Computational Materials Engineering Expert Group (ICMEg) aims at developing a global open standard for information exchange among multiscale simulation tools. The overall aim is to build up a scientific network of stakeholders interested in boosting ICME into industrial applications. The stakeholders will benefit from sharing knowledge and best practice. A deeper understanding across the communities of materials scientists, information-technology engineers and industrial users will be promoted.

The main role of the IMDEA Materials Institute in the ICMEG project is not only to provide sand-box scenarios and industrial use cases, but also to contribute with its general expertise and network of contacts.

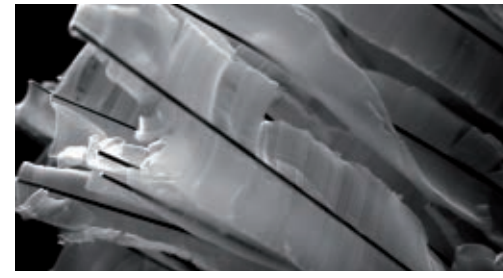
NFRP

"Nano-Engineered Fibre-Reinforced Polymers"

Funding: **Marie Curie Action career integration grants (CIGs), EU Seventh Framework Programme for Research (FP7)**
Duration: **2013-2017**
Principal Investigator: **Dr. R. Guzmán de Villoria**

Fibre-reinforced polymers (FRP) present outstanding specific mechanical properties and are widely used in structural applications, particularly in aerospace. They are made of carbon-fibre "plies" which are held together by a polymer. This architecture hinders the through-the-thickness electrical conductivity and, in addition, the polymer can crack easily, which results in the delamination of the plies. Moreover, composites should withstand the effect of lightning strikes, electromagnetic interferences and electrostatic discharge, among others.

The NFRP project aims at developing a novel nano-architecture to enhance the mechanical and electrical properties of the aerospace composites in the through-the-thickness direction. This nano-architecture will also act as a sensing system, enabling damage detection and localisation by resistive-heating based non-destructive evaluation. In summary, the nano-engineered composite will behave as an intrinsically multifunctional material, with improved mechanical and multifunctional properties.

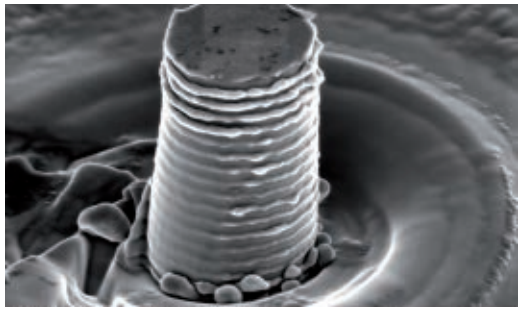


NANOLAM

"High temperature mechanical behaviour of metal/ceramic nanolaminate composites"

Funding: **Materials World Network (supported by the Spanish Ministry of Economy and Competitiveness and National Science Foundation of the United States)**
Partners: IMDEA Materials Institute (Spain), Arizona State University (USA) and Los Alamos National Laboratory (USA)
Duration: **2013-2015**
Principal Investigator: **Dr. J. M. Molina-Aldareguía**

Multilayered materials at the nanoscale enjoy significant potential in structural applications not only because of their extremely high strength, but also their fatigue, wear and thermal resistance. These properties – which are significantly higher than those reported in bulk materials – arise because of their higher interfacial area and notably smaller length scale. This can lead to new types of deformation mechanisms that are



rather different from those observed in bulk systems. It is clear that fundamental research on the mechanical behaviour of metal/ceramic multilayers at the nanoscale is necessary for successful implementation of these materials in engineering applications.

NANOLAM is an international collaborative research project that seeks to address several new topics in the area of nanoscale multilayers: (i) synthesis and microstructural characterisation of ultra-thick Al/SiC nanolaminates with minimal contribution from the underlying substrate; (ii) evolution of damage in ultra-thick nanolaminates under tensile and fatigue loading; (iii) high temperature nanoindentation and micropillar compression to elucidate creep mechanisms, (iv) continuum and atomistic simulations to rationalise experimental findings. State-of-the-art synthesis, characterisation, mechanical testing and simulation techniques will be employed in the research.

The IMDEA Materials Institute will perform nanomechanical testing at high temperatures and will complement the multiscale modeling effort at Los Alamos National Laboratory.

GOBIERNO DE ESPAÑA | MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

NETHIPEC

"Next Generation High Performance Epoxy-based Composites: Green Recycling and Molecular-level Fire Retardancy"

Funding: **Spanish Ministry of Economy and Competitiveness**
Duration: **2013-2014**
Principal Investigator: **Dr. D.-Y. Wang**

Epoxy resins are one of the most widely used and versatile compounds in the polymeric resins family. The two main limitations identified in many applications are recyclability and flammability. The NETHIPEC project is aimed at understanding the recycling mechanisms of epoxy-based materials and improve their fire retardancy. The objectives of the project involve the two that follow. Firstly, design and development of novel multifunctional high reactivity curing agents that entail controllable functional cross-linking groups on the wall of beta-cyclodextrin structures (easily recyclable at the end of service life). And secondly, improvement of fire retardancy by a synergistic approach that combines molecular-level dispersion, multi-element addition (P, Si, C, O) and gas-condensed phase intumescent fire retardant that relies on the cavity of cyclodextrin (an excellent fire retardant). In parallel, the regeneration of epoxy resins formed by recycled epoxy monomer will be studied. It is expected that the recycled epoxy will provide even higher mechanical properties and better fire retardancy than the parent epoxy.

NANOAL

"Nanostructured Al alloys with improved properties"

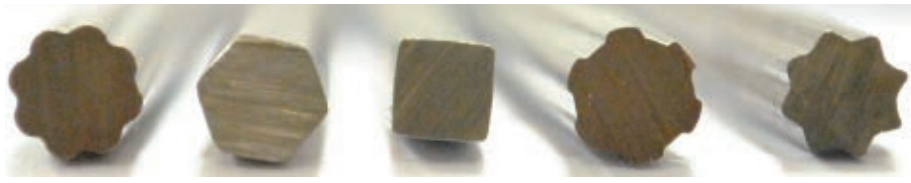
MINISTRY OF EDUCATION AND SCIENCE OF THE RUSSIAN FEDERATION

Funding: **Ministry of Education and Science of the Russian Federation**
Duration: **2013-2014**
Principal Investigator: **Dr. I. Sabirov**

Aluminium alloys play a key role in modern engineering, given that they are the most used non-ferrous metallic material. They are widely used in automotive, aerospace, construction, and electrical engineering, due to their good corrosion resistance and mechanical properties, good machinability, weldability and relatively low cost. It is now well known that nanostructuring of the Al alloys can significantly improve their properties, making them attractive for various structural and functional applications.

NANOAL is an innovative project with a two-fold objective. Firstly, to develop novel processing routes for fabrication of high-strength nanostructured Al alloys with enhanced electrical conductivity in the shape of wires for electrical engineering applications. And secondly, to gain a fundamental understanding of the effect of nanostructuring on the origin of high-strength and enhanced conductivity in Al alloy

The activities of the IMDEA Materials Institute will focus on the physical simulation of deformation processing, as well as on mechanical characterisation of the nanostructured Al alloys.



ECOPVC

"Eco-friendly Fire Retardant PVC Nanocomposites"

CHINA SCHOLARSHIP COUNCIL

Funding: **China Scholarship Council**
Duration: **2013-2017**
Principal Investigator: **Dr. D.-Y. Wang**

PVC is one of the most widely use polymers in industrial applications. ECOPVC aims to develop a series of eco-friendly fire retardant technologies so that PVC may replace the

traditional approach based on antimony oxides (which inflict harm on the environment). Multifunctional and eco-friendly new nanomaterials and nanocarriers will be designed and synthesised in the project to improve fire retardancy of PVC while all other properties are maintained (or even improved). The burning behaviour and flame retardant mechanisms of the new PVC nanocomposites will be fully examined.

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

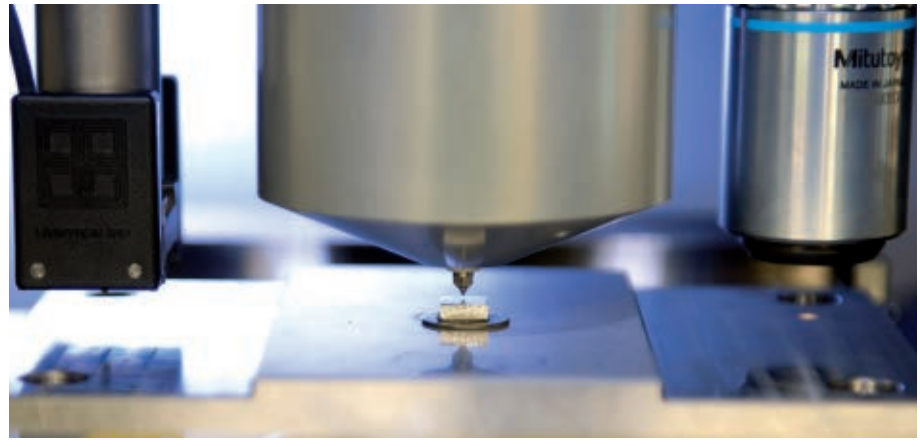
HOTNANOMECH

"Nanomechanical Testing of Strong Solids at High Temperatures"

Funding: **Spanish Ministry of Economy and Competitiveness**
Duration: **2013-2016**
Principal Investigator: **Dr. J. M. Molina-Aldareguía**

The general objective of this project is the development of micromechanical characterisation techniques at high temperature for the study of strong nanoscale multilayered materials. Micropillar compression will be used for testing the deformation and fracture mechanisms of complex strong solids, with negligible size effects, in a wide range of temperatures and strain rates, to obtain the constitutive behaviour of single phases and/or single grains of the bulk material at different orientations.

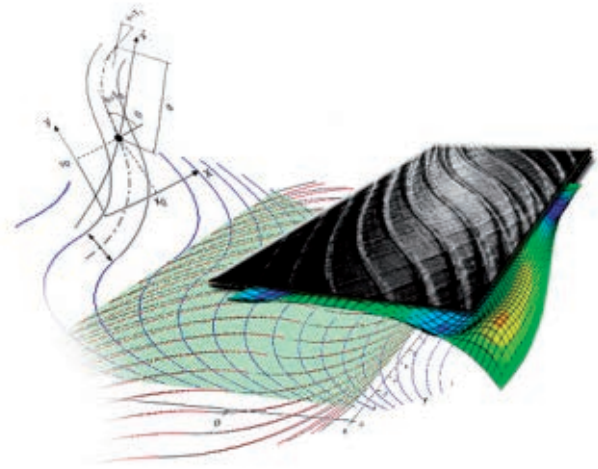
This approach will be applied to two nanolayered material systems of technological relevance: fully-lamellar TiAl intermetallics and nanoscale multilayers. The technique can provide valuable information regarding the macroscopic mechanical behaviour of these materials as a function of layer spacing and orientation across a wide range of temperatures. This information, in combination with multiscale modelling, will contribute to the design and optimisation of the microstructure of these materials.



MUDATCOM

"Multifunctional and Damage Tolerant Composites: Integration of Advanced Carbon NanoFillers and Non-Conventional Laminates"

Funding: **Spanish Ministry of Economy and Competitiveness**
Partners: Technical University of Madrid (Coordinator, Spain), IMDEA Materials Institute (Spain) and University of Girona (Spain)
Duration: **2013-2016**
Principal Investigator: **Dr. J. J. Vilatela**



Fibre-reinforced polymers enjoy the excellent strength and stiffness-to-weight ratio required for lightweight driven structural applications in aerospace. However, several open issues should be addressed in order to consolidate and expand their use in other industrial sectors. These include poor damage tolerance and through-the-thickness properties, as well as low thermal/electrical conductivity. The aim of this coordinated national project is to design new composite laminates by the synergistic combination of smart non-conventional configurations and use of advanced nanofillers such as graphene, nano-platelets and carbon nanotubes. Additionally, new non-destructive evaluation techniques based on thermography will take advantage of the enhancement of thermal/electrical conductivity through the inclusion of nanofillers.

IMDEA Materials will lead the subproject related with the development of new composite materials by means of the inclusion of advanced nanofillers, enhancing the thermal and electrical properties and adding sensing capabilities.

Other research projects currently running at the IMDEA Materials Institute are:

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

Funding: **NMP, EU Seventh Framework Programme for Research (FP7)**
Partners: Consortium of 26 European partners coordinated by the European Space Agency (France)
Duration: **2012-2016**
Principal Investigator: **Dr. J. M. Molina-Aldareguía and Dr. M. T. Pérez-Prado**

MUFIN "Multifunctional fibre nanocomposites"

Funding: **Marie Curie Action career integration grants (CIGs), EU Seventh Framework Programme for Research (FP7)**
Duration: **2012-2016**
Principal Investigator: **Dr. J. J. Vilatela**

SIMSCREEN "Simulation for screening properties of materials"

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

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

Funding: **Marie Curie Action career integration grants (CIGs), EU Seventh Framework Programme for Research (FP7)**
Duration: **2012-2016**
Principal Investigator: **Dr. D.-Y. Wang**

ITER PCR "Mechanical analysis ITER Pre-Compression Rings"

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

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

Funding: **Marie Curie Action career integration grants (CIGs), EU Seventh Framework Programme for Research (FP7)**
Duration: **2012-2016**
Principal Investigator: **Dr. S. Milenkovic**

VMD "Virtual Materials Design"

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

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**
Duration: **2012-2015**
Principal Investigator: **Dr. S. Milenkovic**

Pre-HITMAAS "High temperature material/solution selection"

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

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

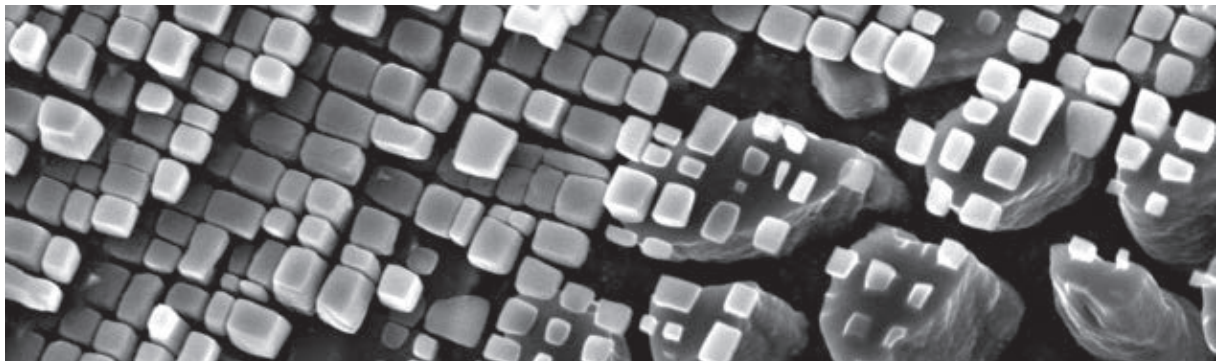
Funding: **AIRBUS OPERATIONS S.L. (Spain)**
Duration: **2012-2013**
Principal Investigators: **Dr. C. S. Lopes and Dr. C. González**

ScreenPTK "Screening of phase transformation kinetics of Ti alloys by diffusion multiple approach and mesoscale modeling"

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

HIFIRE "High performance environmentally friendly fire retardant epoxy nanocomposites"

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



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 career integration grants (CIGs), EU Seventh Framework Programme for Research (FP7)**
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, EU Seventh Framework Programme for Research (FP7)**
Partners: Centre National de la Recherche Scientifique (Coordinator, France), University of Oviedo (Spain), Universidad Politecnica de Madrid (Spain), Ecole des Mines de Paris-ARMINES (France), Czech Technical University in Prague (Czech Republic), Universita degli Studi di Cagliari (Italy), University of Tartu (Estoni), Uppsala University (Sweden), IMDEA Materials Institute (Spain) and Los Alamos National Laboratory (USA).
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, EU Seventh Framework Programme for Research (FP7)**
Partners: Fundació CTM Centre Tecnològic (Coordinator, Spain), ThyssenKrupp Steel Europe AG (Germany), aArcelor-Mittal (Belgium), 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, EU Seventh Framework Programme for Research (FP7) (Coordinated call with Russia)**
EU Partners: Technical University of Denmark (Coordinator, 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 (Coordinator), Ufa State Aviation Technical University, Institute of Strength Physics and Materials Science, Scientific-Industrial Enterprise "Metal", NanoMeT Ltd..
Duration: **2011-2014**
Principal Investigators: **Dr. J. Segurado and Dr. I. Sabirov**

SEMICURED ("Semi-cured products manufacturing")

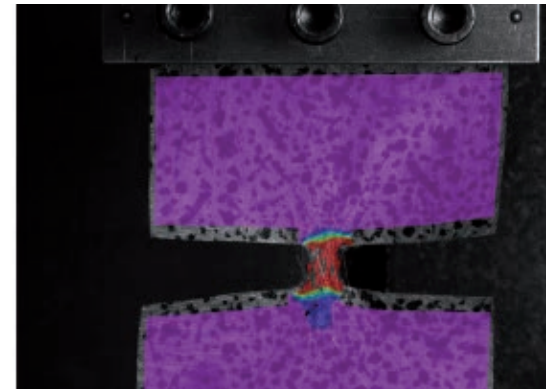
Funding: **Airbus Operations S. L. (Spain)**
Duration: **2011-2012**
Principal Investigator: **Dr. C. González**

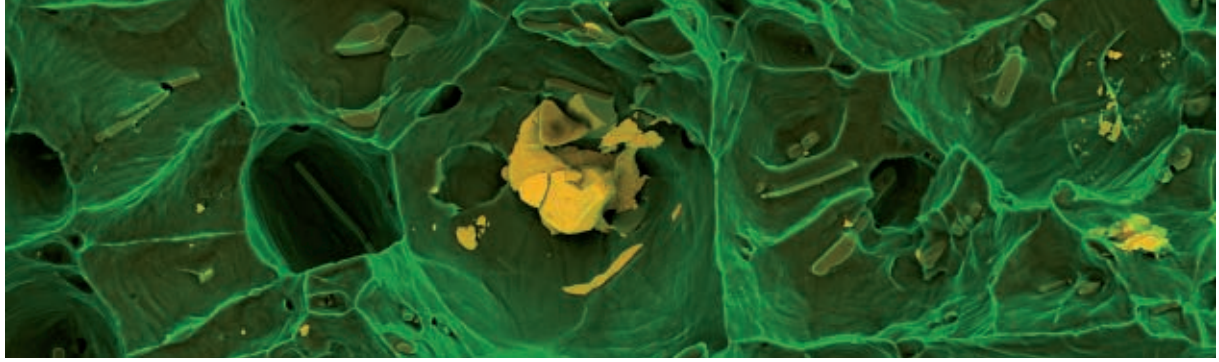
MAGMAN "Analysis of the microstructural evolution and mechanical behaviour of Mg-Mn-rare earth alloys"

Funding: **Materials World Network (supported by Spanish Ministry of Economy and Competitiveness and National Science Foundation of the United States)**
Partners: IMDEA Materials Institute (Spain), Technical University of Madrid (Spain) 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: **China Scholarship Council (China)**
Duration: **2011-2014**
Principal Investigators: **Dr. Y. Cui and Prof. J. LLorca**

MASID "Modelling of advanced semiconductor integrated devices

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

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

Funding: **China 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, EU Seventh Framework Programme for Research (FP7)**
Partners: Consortium of 16 European partners coordinated by Coexpair (France)
Duration: **2010-2012**
Principal Investigator: **Dr. C. González**

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

Funding: **Airbus Operations**
Duration: **2010-2014**
Principal Investigator: **Dr. C. González**

CAJAL BLUE BRAIN

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

VANCAST "Next generation nozzle guide vanes"

Funding: **ERA-Matera+, EU Seventh Framework Programme for Research (FP7)**
Partners: IMDEA Materials Institute (Coordinator, Spain), Industria de Turbo Propulsores (Spain), Precicast Bilbao (spain), Calcom-ESI (Switzerland), University of Applied Sciences of Switwerland (Switzerland) and Precicast Novazzano (Italy)
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+, EU Seventh Framework Programme for Research (FP7)**
Partners: IMDEA Materials Institute (Coordinator, Spain), Université de Liège (Belgium), CENAERO (Belgium), Centre de Recherche Public Henri Tudor (luxembourg) and e-Xstream Engineering (USA)
Duration: **2010-2013**
Principal Investigator: **Dr. A. Jérusalem**

LIMEDU "High Strength Light Metals with Increased Ductility"

Funding: **ERA-Matera+, EU Seventh Framework Programme for Research (FP7)**
Partners: IMDEA Materials Institute (Coordinator, Spain), Polish Academy of Science (Poland) and Carlos III University of Madrid (Spain)
Duration: **2010-2013**
Principal Investigator: **Dr. I. Sabirov**

HOTNANO "High temperature nanoindentation"

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

ESTRUMAT "Advanced structural materials"

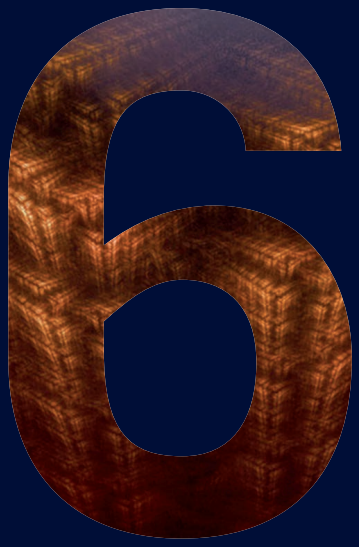
Funding: **Regional Government of Madrid, General Direction for Research**
Partners: Rey Juan Carlos University (Coordinator, Spain), IMDEA Materials Institute (Spain), Polytechnic University of Madrid (Spain), Carlos III University of Madrid (Spain) and Complutense University of Madrid (Spain)
Duration: **2010-2013**

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

MAAXIMUS "More affordable aircraft structure lifecycle through extended, integrated, & mature numerical sizing"

Funding: **Transport, EU Seventh Framework Programme for Research (FP7)**
Partners: Consortium of 57 European partners from 18 countries coordinated by AIRBUS OPERATIONS GmbH
Duration: **2008-2016**
Principal Investigator: **Prof. J. LLorca**

dissemination of results



publications

6.1 Publications

1. J. M Torralba, L. Fuentes-Pacheco, N. García-Rodriguez, M. Campos, *Development of high performance powder metallurgy steels by high-energy milling*, **Advanced Powder Technology 24**, 813–817, 2013.

2. N-J Kang, D-Y Wang, B. Kutlu, P-C Zhao, A. Leuteritz, U. Wagenknecht, G. Heinrich, *A New Approach to Reducing the Flammability of Layered Double Hydroxide (LDH)-Based Polymer Composites: Preparation and Characterization of Dye Structure-Intercalated LDH and Its Effect on the Flammability of Polypropylene-Grafted Maleic Anhydride/d-LDH Composites*, **ACS Applied Materials and Interfaces 5**, 8991–8997, 2013.

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4. S. Lotfian, M. Rodríguez, K. E. Yazzie, N. Chawla, J. LLorca, J. M. Molina-Aldareguia, *High temperature micropillar compression of Al/SiC nanoscale multilayers*, **Acta Materialia 61**, 4439-4451, 2013.

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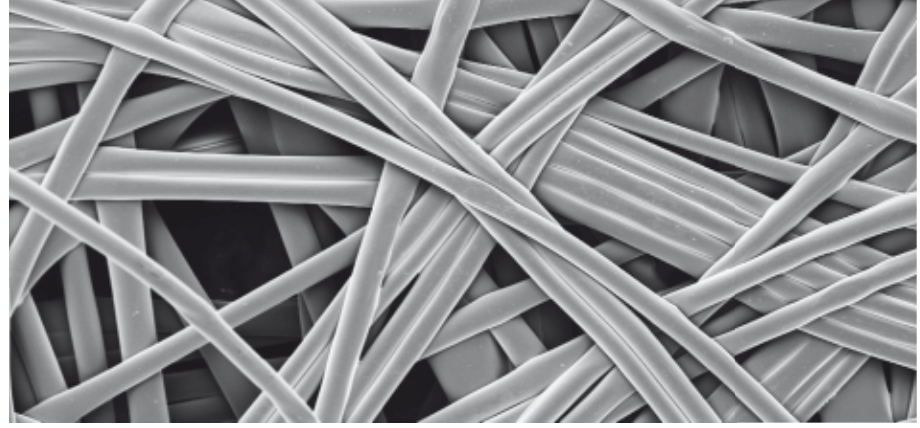

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6.2 Patents

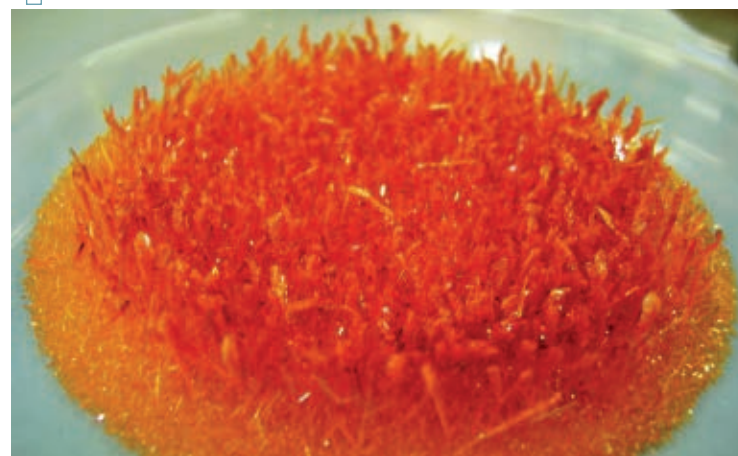
1. *"Halogen free flame retardant polymeric composition comprising a modified layered double hydroxide nanofiller"*. D. Y. Wang, N. Kang, E. Kalali, C. Li, X. Zhao, Application PCT/EP2013/067696 (27 August 2013).

2. *"A halogen free flame retardant epoxy resin composition"*. D. Y. Wang, N. Kang, X. Zhao, Application PCT/EP2013/063658 (28 June 2013).

3. *"Thermoset curing through resistive heating of nanocarbons"*. J. J. Vilatela, B. Mas, J. P. Fernández-Vázquez, H. Bunyan, J. Duval, Application PCT/EP2013/055659 (19 March 2013). 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. ES2382851 (19 November 2010). Joint ownership with Future Fibres rigging systems S.L.

patents



6.3 International Conferences

6.3.1 Invited and Plenary talks

1. *"High temperature mechanical properties of nanoscale metallic multilayers"*. J. LLorca, **International Workshop on Nanostructured Ti-based Alloys for Medical Applications: Mechanical Properties and Biocompatibility**, Ein Gedi, Israel, January 2013.

2. *"Environmental Friendly Fire retardants"* D. Y. Wang, **Workshop of United Nations Industrial Development Organization (UNIDO)**, Vienna, Austria, January 2013.

3. *"High temperature mechanical behaviour of Nanoscale Multilayers"*. J. M. Molina-Aldareguia, S. Lotfian, M. Monclus, J. LLorca, N. Chawla, I. Beyerlein, N. Mara, **TMS Annual Meeting & Exhibition 2013**, San Antonio, USA, March 2013.

4. *"High temperature mechanical behavior of Nanoscale Multilayers"*. J. M. Molina-Aldareguia, S. Lotfian, M. Monclus, J. LLorca, N. Chawla, I. Beyerlein, N. Mara, **Nanobrücken-Dresden: A Nanomechanical Testing Workshop & Hysitron User Meeting**, Dresden, Germany, March 2013.

5. *"In-Situ Analysis of the deformation mechanisms in Mg alloys between 50-250°C"*. C. J. Boehlert, Z. Chen, A. Chakkedath, M. T. Pérez-Prado, J. LLorca, I. Gutiérrez-Urrutia, S. Yi, D. Letzig, J. Bohlen, **TMS Annual Meeting & Exhibition 2013**, San Antonio, USA, March 2013.

6. *"Nanocomposites and Nano-architectures"*. R. G. de Villoria, **Technological Foresight Workshop, Center for Engineering and Industrial Development (CIDESI)**, NC, U.S.A. March 2013.

7. *"High temperature mechanical characterization and modeling of Al/SiC nanolaminates"*. J. M. Molina-Aldareguia, S. Lotfian, K. Yazzie, H. Xie, J. LLorca, J. K. Baldwin, A. Misra, N. Chawla, **TMS Annual Meeting & Exhibition 2013**, San Antonio, USA, March 2013.

8. *"Simulating is believing: the role of simulation in nanomechanics"*. J. LLorca, **Workshop on Nanomaterials and Nanomechanics**, Universidad Rey Juan Carlos, Madrid, Spain, April 2013.

9. *"High strength metallic conductors with enhanced conductivity"*. I. Sabirov, **Second International Conference on Materials for Energy (EnMat II)**, Karlsruhe, Germany, May 2013.

10. *"Advanced PM Materials and Processes"*, J. M. Torralba, **Werstoffsymposium Pulvermetallurgie in Dresden**, Dresden, Germany, May 2013.

11. *"Fire Retardant Polymer Materials"*, D. Y. Wang, **Asia-Europe Symposium on Processing and Properties of Reinforced Polymers (AESP6)**, Wuhan, China, June 2013.

12. *"Multicale materials modelling: success stories and current challenges"*. J. LLorca, **International Workshop on New Horizons in Materials Mechanics**, Lyngby, Denmark, June 2013.

13. *"Hierarchical Mechanisms of Energy Dissipation at the nm and μm Scale During Fracture of Advanced Fiber-reinforced Composites"*. F. Sket, L .P. Canal, R. Guzmán de Villoria, J. M. Molina Aldareguia, C. González, J. LLorca, **7th International Conference on Materials for Advanced Technologies (ICMAT2013)**, Singapore, July 2013.

14. *"New Ideas on Fire Retardantcy of Polymer Nanocomposites"*. D. Y. Wang, **Eurofillers 2013**, Bratislava, Slovakia, August 2013.

15. *"Fire Retardantcy of Polymer Nanocomposites"*. D. Y. Wang, **EUROMAT 2013**, Seville, Spain, September 2013.

16. *"Microstructural development of a HIP'ed γ-TiAl intermetallic alloy by means of heat treatments"*. R. Muñoz-Moreno, M. T. Pérez-Prado, E. M. Ruiz-Navas, J. M. Torralba, **EURO-PM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013

17. *"Discrete (MD) and continuum (DD) simulations of void growth in single crystals"*. O. Rodríguez, J. Segurado, H-J. Chang, J. LLorca, **XII International Conference on Computational Plasticity. Fundamentals and Applications (Complas XII)**, Barcelona, Spain, September 2013.

18. *"Latent hardening size effect in small-scale plasticity"*. L. Bardella, J. Segurado, A. Panteghini, J. LLorca, **XII International Conference on Computational Plasticity. Fundamentals and Applications (Complas XII)**, Barcelona, Spain, September 2013.

19. *"Multiscale design of nano-engineered structural composites"*. J. LLorca, C. González, C. S. Lopes, **Composites Week**, Leuven, September 2013.

20. *"Integrated Computational Materials Techniques: from Quantitative Modeling to Virtual Alloy Design"*. Y. Cui, X-G Lu, G. Xu, X. Tao, Y. Chen, D-W Lee, **2013 International Forum of New Materials Development Trends**, Chengdu, China, September 2013.

21. *"High Temperature Mechanical Behaviour of Al/SiC Multilayers"*. J. M. Molina-Aldareguia, S. Lotfian, H. Y. Xie, C. Mayer, N. Chawla, J. LLorca, A. Misra, **Nanoscale Multilayers'13**, Madrid, Spain, October 2013.

22. *"Anisotropy of the Mechanical Response of Al/SiC Multilayers"*. J. LLorca, J. M. Molina Aldareguia, S. Lotfian, C. Mayer, N. Chawla, A. Misra, **Nanoscale Multilayers'13**, Madrid, Spain, October 2013.

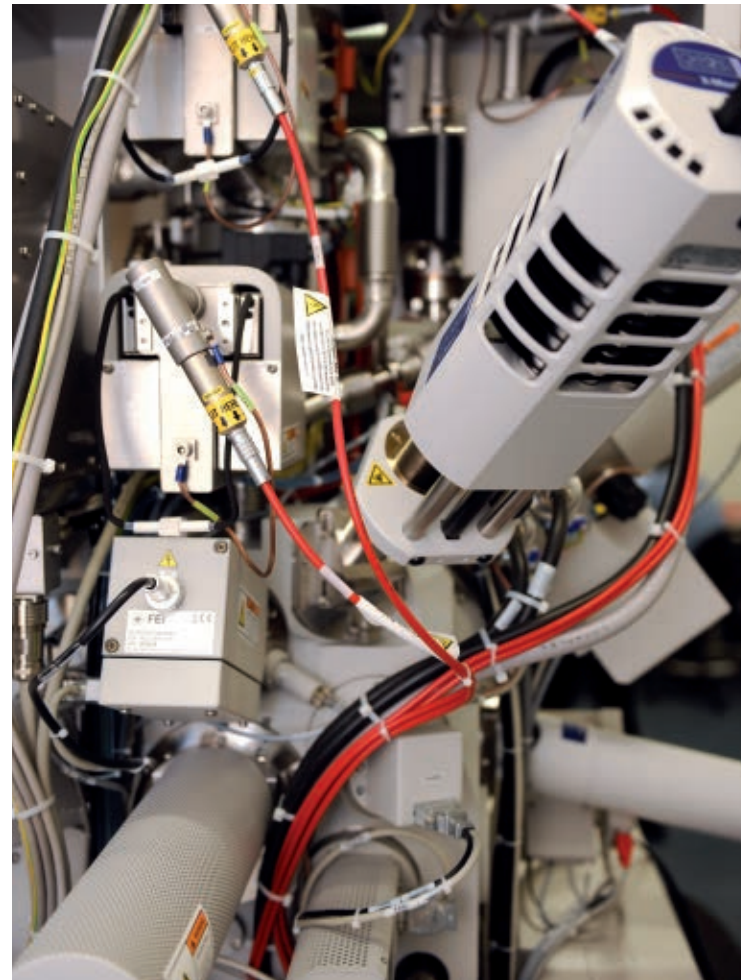
23. *"High-temperature Mechanical Properties of Physical Vapourdeposited (PVD) and Accumulative Roll-bonded (ARB) Cu/Nb Nanoscale Metallic Multilayers"*, M. Monclús, I. Beyerlein, N. Mara, S. Zheng, T. Polcar, J. LLorca, J. M. Molina-Aldareguia, **Nanoscale Multilayers'13**, Madrid, Spain, October 2013.

24. *"High temperature mechanical behavior of nanoscale Multilayers"*. J. M. Molina-Aldareguia, **Nanomechanical Testing in Materials Research and Development IV,** Olhão, Portugal, October 2013.

25. *"Multiscale Engineering of Carbon Nanotube fibres"*. J. J. Vilatela, **2013 Fibre Society Fall Conference**, Clemson, USA, October 2013.

26. *"High fidelity simulations of the mechanical behaviour of composite materials and structures for wind turbines"*. J. LLorca, **Asia Future Energy Forum**, Singapore, October 2013.

27. *"Formability of ultra-fine grained metallic materials"*. I. Sabirov, E. C. Moreno-Valle, M. Kulczyk, W. Pachla, **International Conference on Processing and Manufacturing of Advanced Materials (THERMEC 2013)**, Las Vegas, USA, December 2013.



6.3.2 Regular Contributions

1. *"Anisotropy of mechanical properties in ultra-fine grained commercially pure Ti for dentals implants"*. I. Sabirov, J. Segurado, R.Z. Valiev, D.V. Gunderov, N. Enikeev, J. LLorca. **International Workshop on Nanostructured Titanium based alloys for medical applications: Mechanical Properties and Biocompatibility**, Ein Gedi, Israel, January 2013.

2. *"Mechanical Characterization of Nanolayered Al/SiC Composites by High Temperature Nanoindentation"*. S. Lotfian, J. M. Molina-Aldareguia, K.E. Yazzie, J. LLorca, A. Misra, N. Chawla, **TMS Annual Meeting & Exhibition 2013**, San Antonio, USA, March 2013.

3. *"High Temperature Nanoindentation of Microstructural Constituents in a Sn-rich Pb-Free Solder"*. J. Molina-Aldareguia, S. Lotfian, K. Yazzie, J. LLorca, N. Chawla, **TMS Annual Meeting & Exhibition 2013**, San Antonio, USA, March 2013.

4. *"Damage mechanisms of 3D woven hybrid composites loaded in tension, testing, inspection and simulation"*. R. Muñoz, C. González, J. LLorca, **6th International Conference on Composite Testing and Model Identification (CompTest2013)**, Aalborg, Denmark, April 2013.

5. *"Biaxial deformation behavior and enhanced formability of ultrafine-grained pure copper"*. E. C. Moreno-Valle, M. A. Monclus, J. M. Molina-Aldareguia, N. Enikeev, I. Sabirov, **The 16th Annual ESAFORM Conference on Material Forming (ESAFORM 2013)**, Aveiro, Portugal, April, 2013.

6. *"X-Ray Tomography Assessment of Damage during Tensile Deformation of ±45° Carbon Fiber Laminates"*. F. Sket, A. Enfedaque, C. Alton, C. González, J. M. Molina Aldareguía, J. LLorca, **6th International Conference on Composite Testing and Model Identification (CompTest2013)**, Aalborg, Denmark, April 2013.

7. *"Development of a Crystal Plasticity Model for Mg Alloys"*. V. Herrera, J. Segurado, J. LLorca, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May 2013.

8. *"Measuring the Critical Resolved Shear Stresses in Mg Alloys by Instrumented Nanoindentation"*. R. Sanchez, M. T. Pérez-Prado, J. Segurado, I. Gutierrez, J. LLorca, J. M. Molina-Aldareguia, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May 2013.

9. *"3D Polycrystalline Continuum Model of Deformation Mechanisms in Rolled Magnesium Alloys"*. A. Fernández, M. T. Pérez-Prado, A. Jeérusalem, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys,** Madrid, Spain, May 2013.

10. "*Stabilization of an HCP-Li Phase at Room Temperature in a Mg-Li Alloy by High Pressure Torsion"*. B. Srinivasarao, I. Gutiérrez-Urrutia, A. P. Zhilyaev, M. T. Pérez-Prado, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May 2013.

11. *"Three Dimensional EBSD Characterization of Deformation Twinning in Mg Alloys: Application to AZ31"*. I. Gutiérrez-Urrutia, A. Fernández, A. Khorashadizadeh, A. Jérusalem, M. T. Pérez-Prado, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May 201

12. *"Influence of the Extrusion Conditions and the Neodymium Content on the 'Microstructure, the Texture and the Deformation Behaviour of Magnesium-manganese Alloys"*. P. Hidalgo-Manrique, S. Yi, J. Bohlen, D. Letzig, M. T. Pérez-Prado, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May 2013.

13. *"The Effect of Neodymium on the Deformation Behavior of Extruded Mg-1Mn (wt%)"* A. Chakkedath, Z. Chen, C. J. Boehlert, I. Gutiérrez-Urrutia, J. LLorca, J. Bohlen, S. Yi, D. Letzig, M. T. Pérez-Prado, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May 2013.

14. *ωIn-situ analysis of the deformation mechanisms in Mg alloys between 50-250°CωZ.* Chen, A. Chakkedath, I. Gutiérrez-Urrutia, J. Bohlen, S. Yi, D. Letzig, J. LLorca, M. T. Pérez-Prado, C. J. Boehlert, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May 2013.

15. *"Evaluating the plastic anisotropy of AZ31 using microscopy techniques"*. M. T. Pérez-Prado, Z. Chen, J. LLorca, C. J. Boehlert, **International Workshop on Processing-Microstructure-Mechanical Property of Magnesium Alloys**, Madrid, Spain, May, 2013.

16. *"Integrated Computational Alloy Design for Advanced Rare Metal Materials: Thermo-Kinetic & Landau/Phase Field Modeling"*. Y. Cui, **XLII International Conference on Computer Coupling of Phase Diagrams and Thermochemistry (CALPHAD XLII)**, San Sebastian, Spain, May 2013.

17. *"Atomistic modeling and simulation of arsenic diffusion including mobile arsenic clusters"*. I. Martin-Bragado, N. Zographos, P. Castrillo, **E-MRS 2013**, Strasbourg, France, May 2013.

18. *"Lattice Kinetic Monte Carlo modeling of germanium solid phase epitaxial growth"*. J. L. Gómez-Selles, B. L. Darby, K. S. Jones, I. Martin-Bragado, **E-MRS 2013**, Strasbourg, France, May, 2013.

19. *"Atomistic modeling of stressed solid phase epitaxial regrowth of silicon using a lattice kinetic Monte Carlo approach"*. B. Sklenard, I. Martin-Bragado, J. C. Barbe, P. Batude, P. Rivallin, C. Tavernier, S. Cristoloveanu, **E-MRS 2013**, Strasbourg, France, May 2013.

20. *"Computational micromechanical model of ply failure: Matrix cracking, delamination and crack density"*. D. F. Mora, C. Gonzalez, C. S. Lopes, **International Conference on Computational Modeling of Fracture and Failure in Materials and Structures 2013**, **(CFRAC 2013)**, Prague, Czech, June 2013.

21. *"Variable stiffness composite panels. Modeling methodology and prediction of the failure behaviour"*. O. Falco, J. Mayugo, C. S. Lopes, N. Gascons, J. Costa, **17th International Conference on Composite Structures (ICCS17)**, Porto, Portugal, June 2013.

22. *"Dispersed CFRP Laminates for Damage Tolerant Aeronautical Structures"*. T. A. Sebaey, C. S. Lopes, N. Blanco, J. Costa, **17th International Conference on Composite Structures (ICCS17)**, Porto, Portugal, June 2013.

23. *"Impact simulations in variable-stiffness panels"*. A. R. Melro, C. S. Lopes, P. P. Camanho, **17th International Conference on Composite Structures (ICCS17)**, Porto, Portugal, June, 2013.

24. *"High temperature mechanical behavior of Nanoscale Multilayers"*. M. Monclús**, Laboratorio de Microscopías Avanzadas Users Meeting 2013,** Instituto de Nanociencia de Aragon, Zaragoza, Spain, June 2013.

25. *"Graphene activities at IMDEA Materials: synthesis, processing and applications"*. J. J. Vilatela, **Summer Courses UIMP,** Santander, Spain, July 2013.

26. *"Multilayers ballistic systems based on dry fabrics for UERF applications"*. F. Martínez-Hergueta, C. González, J. LLorca, **International Conference of Composite Materials (ICCM19)**, Montreal, Canada, July 2013.

27. *"Resistive heating structural damage detection in nanocomposites"*. R. G. de Villoria, **International Conference of Composite Materials (ICCM19)**, Montreal, Canada, July 2013.

28. "*Damage resistance and damage tolerance of composite laminates with dispersed stacking sequences*". C. S. Lopes, T. A. Sebaey, E. V. González, N. Blanco, J. Costa, **International Conference of Composite Materials (ICCM19)**, Montreal, Canada, July 2013.

29. *"On the use of in-situ SEM testing and simulation to analyze the deformation and failure mechanism in composite materials".* L. P. Canal, C. González, J. Segurado, J. LLorca, **MATCOMP13**, Algeciras, Spain, July 2013.

30. "*Estudio del proceso de infusión de resina por vacio mediante técnicas de correlación digital de imágenes*". J. Vilà, C. González, J. LLorca, **MATCOMP13**, Algeciras, Spain, July 2013.

31. "*Materiales compuestos laminados con refuerzos en orientaciones no-convencionales para una mejora de la tolerancia a impacto de estructuras aeronáuticas*". J. Costa, T. Sebaey, E. V. González, N. Blanco, C. S. Lopes, **MATCOMP13**, Algeciras, Spain, July, 2013.

32. *"Síntesis de Nanotubos de Carbono Verticalmente Alineados para su uso como Refuerzo en Materiales Compuestos"*, R. G. de Villoria, **MATCOMP13**, Algeciras, Spain, July 2013.

33. *"High-velocity impact of 3D woven composites: ballistic curve and failure mechanisms"*. F. Martínez-Hergueta, R. Muñoz, F. Gálvez, C. González, J. LLorca, **7th International Conference on Materials for Advanced Technologies ICMAT 2013**, Singapore, July 2013.

34. *"Interdiffusion and Mobility of f.c.c Co-base Solid Solutions"*, Y. Cui, G. Xu, R. Kato, R. Kainuma, K. Ishida, **International Workshop on Advanced Cobalt-Base Superalloys,** Pommersfelden, Germany, July 2013.

35. *"Biaxial deformation behavior and formability of ultra-fine grained pure Ti"*. E. C. Moreno-Valle, M. A. Monclus, J. M. Molina-Aldareguia, M. Kulczyk, W. Pachla, I. Sabirov, **International Conference on Computational Modelling of Nanostructured Materials)**, Frankfurt am Main, Germany, September, 2013.

36. *"Controlling Debinding and Sintering Atmospheres of Low expansion Invar alloy for μ-PIM"*. J. Hidalgo, A. Jiménez-Morales, T. Barriere, J. C. Gelin, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

37. *"Microstructure and mechanical properties of 7075 aluminum alloy consolidated from a premixed Al-Zn-Mg-Cu powder by hot extrusion"*. M. A. Jabbari Taleghani, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

38. *"Compressibility characteristics of a nanostructured 7075 aluminum alloy powder produced by high-energy milling"*. M. A. Jabbari Taleghani, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

39. *"The microstructural evolution of a premixed Al-Zn-Mg-Cu powder through high-energy milling and subsequent isothermal annealing"*. M. A. Jabbari Taleghani, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

40. *"The effect of mechanical milling on the compressibility of a pre-alloyed Mg-Al-Zn powder"*. M. A. Jabbari Taleghani, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

41. *"Introduction of Oxidation-Sensitive Elements in Low Alloyed Steels using the Master Alloy Route: Key Aspects for Success"*. R. Oro, M. Campos, C. Gierl, H. Danninger, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

42. *"New alloying systems for PM-steels: opportunities for the Mn-Si master alloys"*. R. Oro, M.

Campos, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association, Gotteborg**, Sweden, September, 2013.

43. *"Feedstock development based on eco-friendly binder system for powder injection molding"*. C. Abajo, J. Hidalgo, A. Jiménez-Morales, J. M. Torralba, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

44. *"Lean steels modified with a new Cu base master alloy: influence of process parameters in dimensional and sintering behavior"*, E. Bernardo, M. Campos, J. M. Torralba, C. Gier, H. Danninger, R. Frykholm, **EUROPM'2013, European Powder Metallurgy Association**, Gotteborg, Sweden, September 2013.

45. *"Local deformation behavior and mechanical properties of individual phases in a quenched and partitioned steel"*. I. de Diego-Calderon, D. De Knijf, M. A. Monclus, J. M. Molina-Aldareguia, C. Fojer, I. Sabirov, R. Petrov, **EUROMAT 2013**, Seville, Spain, September 2013.

46. *"Solidification microstructure of Ni-based superalloys"*. M. Rahimian, I. Sabirov, S. Milenkovic, **EUROMAT 2013**, Seville, Spain, September 2013.

47. *"Multiscale modeling of deformation of polycrystalline nanostructured Ti"*. J. LLorca, J. Segurado, A. Ridruejo, **EUROMAT 2013**, Seville, Spain, September 2013.

48. *"Temperature dependent size effects in LiF [111] single crystals"*. R. S. Arnedo, J. Wheeler, J. M. Molina-Aldareguia, C. Hyung-Jun, J. Segurado, J. Michler, J. LLorca, **EUROMAT 2013**, Seville, Spain, September 2013.

49. *"High-temperature mechanical properties and microstructure correlation of physical vapour-deposited and accumulative roll-bonded Cu/Nb nanoscale multilayers"*. J. Molina-Aldareguia, M. Monclús, T. Polcar, N. Mara, I. Beyerlein, J. LLorca, **EUROMAT 2013**, Seville, Spain, September 2013.

50. *"Local deformation behavior and mechanical properties of individual phases in a quenched and partitioned Steel"*. Irene De Diego Calderon, Dorien Knejf, M. Monclú, J. Molina-Aldareguia, C. Fojer, I. Sabirov, R. Petrov, **EUROMAT 2013**, Seville, Spain, September 2013.

51. *"3D Damage characterisation during sequential tensile loading of a multidirectional carbon fibre reinforced epoxy laminate"*, M. Rodríguez-Hortala, G. Requena, F. Sket, J. Molina-Aldareguia, E. Maire, L.Salvo, M. Scheel, **EUROMAT 2013**, Seville, Spain, September 2013.

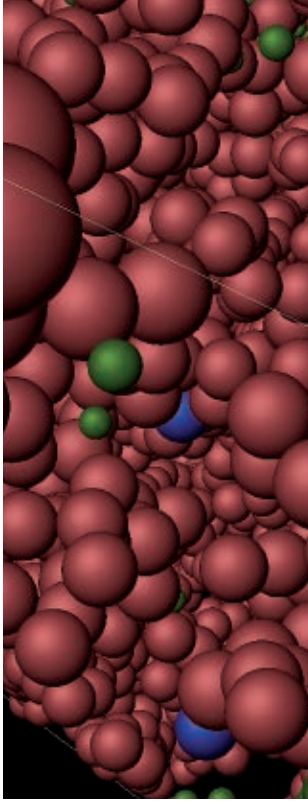
52. *"An XFEM Implementation for Massively Parallel Simulations of Composites Fracture"*, G. Vigueras, C. C. Samaniego-Alvarado, E. Casoni, G. Houzeaux, F. Sket, J. Molina-Aldareguia, A. Makradi, M. Vázquez, A. Jérusalem, **EUROMAT 2013**, Seville, Spain, September 2013.

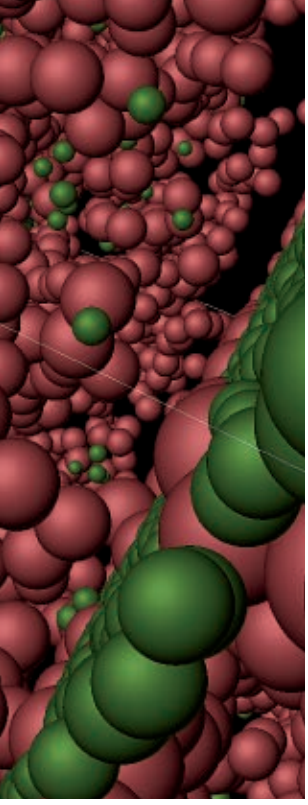
53. *"Effect of interface properties on the compressive behaviour of Al/SiC nanolaminates at high temperature"*, S. Lotfian, M. Rodríguez, H. Xie, C. Mayer, N. Chawla, J. LLorca, A. Misra, J. Molina-Aldareguia, **EUROMAT 2013**, Sevilla, Spain, September 2013.

54. *"Temperature Dependent Size Effects in LiF [111] Single Crystals"*, R. Soler Arnedo, J. Wheeler, J. M. Molina-Aldareguia, C. Hyung-Jun, J. Segurado, J. Michler, J. LLorca, **EUROMAT 2013**, Seville, Spain, September 2013.

55. *"X-ray tomographic investigation of damage evolution of sequential tensile deformation of ±45° plain and open hole carbon fibre laminates"*. F. Sket, A. Enfedaque, C. Alton, C. González, J. LLorca, **EUROMAT 2013**, Seville, Spain, September, 2013.

56. *"Application of in situ X-ray microtomography to creep damage studies"*. A. Borbely, K. Dzieciol, F. Sket, **EUROMAT 2013**, Seville, Spain, September 2013.





57. *"Improved curing of epoxy composites through the addition of nanocarbons"*. B. Mas, J. P. Fernández-Blázquez, J. J. Vilatela, **EUROMAT 2013**, Seville, Spain, September 2013.

58. *"Mechanical behaviour of the NiAl reinforced with W fibres"*. S. Milenkovic, A. Schneider, **EUROMAT 2013**, Seville, Spain, September 2013.

59. *"Synthesis of ordered B2-NiAl by mechanical alloying"*. A. Varona, S. Milenkovic, **EUROMAT 2013**, Seville, Spain, September 2013.

60. *"High temperature deformation mechanism in Ti4522XD microstructures: An in situ SEM-EBSD experimental study"*. R. Muñoz-Moreno, E. M. Ruiz-Navas, C. J. Boehlert, M. T. Pérez-Prado, **EUROMAT 2013**, Seville, Spain, September 2013.

61. *"Optimization of eco-friendly binary binder system for powder injection molding"*. C. Abajo, J. Hidalgo, A. Jiménez-Morales, J. M. Torralba, **EUROMAT 2013**, Seville, Spain, September 2013.

62. *"Wettability study of liquid promoters for improved liquid phase sintering process of steels"*. E. Bernardo, R. Oro, M. Campos, J. M. Torralba, **EUROMAT 2013**, Seville, Spain, September 2013.

63. *"Development and microstructural characterization of nanostructured Fe–Cr–Al–W ODS alloys"*. N. García-Rodríguez, M. Campos, J. M. Torralba, M. H. Berger, Y. Bienvenu, **EUROMAT 2013**, Seville, Spain, September 2013.

64. *"Modification of a powder metallurgy ϒ-TiAl alloy microstructure by heat treatments"*. R. Muñoz-Moreno, M. T. Pérez-Prado, E. M. Ruiz-Navas, J. M. Torralba, **EUROMAT 2013**, Seville, Spain, September 2013.

65. *"Compressibility behavior of an atomized, pre-alloyed Mg-Al-Zn powder"*. M. A. Jabbari Taleghani, J. M. Torralba, **EUROMAT 2013**, Seville, Spain, September, 2013.

66. *"Mapping the Laves phases in Ca-Mg-Cu-Ni system for lightweight hydrogen storage materials: Diffusion Multiple Approach & CALPHAD Method"*. G. Xu, Y. Chen, Y. Cui, **EUROMAT 2013**, Seville, Spain, September 2013.

67. *"Object Kinetic Monte Carlo Simulator for damage irradiation evolution and defect diffusion in generic alloy"*. I. Dopico, P. Castrillo, I. Martin-Bragado, **EUROMAT 2013**, Seville, Spain, September 2013.

68. *"Simulation of the deformation of polycrystalline nanostructured Ti by computational homogenization"*. J. Segurado, D. Rodriguez, H. Ehteshami, V. Herrera, J. LLorca, **International Conference on Computational Modelling of Nanostructured Materials**, Frankfurt am Main, Germany, September 2013.

69. *"Synchrotron X-ray microtomography: applications to material science"*. F. Sket, **ALBA user meeting and VI AUSE Conference,**, Cerdanyola de Vallès, Spain, September, 2013.

70. *"Comportamiento mecánico a alta temperatura de nanolaminados"*. J. M. Molina-Aldareguia, **Seminario de Nanomecánica y Nanomateriales, Universidad Rey Juan Carlos**, Móstoles, Spain, April 2013.

71. *"Multiscale modeling of a small punch test on nanostructured CP titanium"*. A. Ridruejo, J. Segurado, I. Sabirov, J. LLorca, **XII International Conference on Computational Plasticity. Fundamentals and Applications (Complas XII)**, Barcelona, Spain, September 2013.

72. *"Latent hardening size effect in small-scale plasticity"*. L. Bardella, J. Segurado, A. Panteghini, J. LLorca, **XII International Conference on Computational Plasticity. Fundamentals and Applications (Complas XII)**, Barcelona, Spain, September 2013.

73. *"An XFEM-CZM Implementation for Large Scale Parallel Composites Fracture Simulations"*. G. Vigueras, C. Samaniego Alvarado, G.

Houzeaux, F. Sket, J. M. Molina-Aldareguia, A. Makradi, M. Vázquez, A. Jérusalem, **XII International Conference on Computational Plasticity. Fundamentals and Applications (Complas XII)**, Barcelona, Spain, September 2013.

74. *"Photocatalytic water splitting using CNT-inorganic hybrid materials"*. A. Moya, A. Cheveran, S. Marchesan, M. Prato, D. Eder, J. J. Vilatela. **ISACS 12 Conference, Challenges in Chemical Renewable Energy**, Cambridge, UK, September 2013.

75. *"Microstructure and deformation mechanisms of a γ-TiAl intermetallic alloy: An in situ experimental study"*. R. Muñoz-Moreno, E. M. Ruiz-Navas, C. J. Boehlert, J. M. Torralba, M. T. Perez-Prado, **Intermetallics 2013**, Kloster Banz, Germany, October 2013.

76. *"In situ SEM analysis of the deformation and fracture mechanisms of a powder metallurgy g-TiAl alloy"*. R. Muñoz-Moreno, E. M. Ruiz-Navas, C. J. Boehlert, M. T. Perez-Prado, J. M. Torralba, **Intermetallics 2013**, Kloster Banz, Germany, October, 2013.

77. *"Deformation and dynamic recrystallization behaviour of two Fe-Al-Nb alloys reinforced with the Laves phase fibres"*, S. Milenkovic, W. Li, **Intermetallics 2013**, Kloster Banz, Germany, October 2013.

78. *"An object kinetic monte carlo approach to Helium interaction with grain boundaries in Tungsten"*, A. Rivera, G. Valles, R. Gonzalez-Arrabal, J. M. Perlado, I. Martin-Bragado. **Nanoscale Multilayers'13**, Madrid, Spain, October 2013.

79. *"An object kinetic monte carlo model for segregation in multilayered alloys"*. I. Dopico, J. L. Gomez-Selles, P. Castrillo, I. Martin-Bragado, **Nanoscale Multilayers'13**, Madrid, Spain, October 2013.

80. *"Study of Helium-bubbles nucleation at interfaces in Cu/Nb multilayer materials"*. L. Agudo-Merida, I. Martin-Bragado, **Nanoscale Multilayers'13**, Madrid, Spain, October 2013.

81. *"Towards high performance in Powder Metallurgy"*. J. M. Torralba, **International Metallurgical Symposium: 50th Anniversary of CENIM**, Madrid, Spain, October 2013.

82. *"Non destructive evaluation techniques in nanocomposites: a comparative study"* R. G. de Villoria, **Materials Research Society Fall Meeting & Exhibit**, Boston, USA, December 2013.

6.3.3 Membership in Organizing Committees

1. **International Conference on Computer Coupling of Phase Diagrams and Thermochemistry, CALPHAD XLII**. Y. Cui (Member of the National Scientific Committee). San Sebastian, Spain, May 2013.

2. **17th International Conference on Composite Structure, ICCS17**. C. S. Lopes (Organizer of the session Novel Composite Architectures). Porto, Portugal, June 2013.

3. **European Congress and Exhibition on Advanced Materials and Processes, EUROMAT 2013**. J. M. Molina-Aldareguia (Symposium Co-organizer on Mechanical Behavior of Advanced Materials), S. Milenkovic (Symposium Organizer on Intermetallics) and J. M. Torralba (Topic Organizer on Powder and Solution Routes: From Synthesis to Materials). Seville, Spain, September 2013.

4. **Euro PM2013 Congress & Exhibition**. J. M. Torralba. (Programme Committe Member). Gotheborg, Sweden, September 2013.

5. **IUMRS International Conference, IUMRS-ICAM2013**. Y. Cui, (Symposium Organizer on Metal Matrix Composites). Qingdao, China, September 2013.

6. **Nanotube and Graphitic Fibres, 2013 Fibre Society Fall Conference**. J. J. Vilatela (Symposium Organizer). Clemson, USA, October 2013.

7. **8th International Conference on Processing & Manufacturing of advanced Materials, THERMEC 2013**. M. T. Pérez-Prado (Member of the International Advisory Board and of the Scientific Committee). Las Vegas, USA, December 2013

membership in organizing committees

6.4. Hosting and Organisation of International Workshops

international workshops

Four international workshops (devoted to Mg alloys, computational thermodynamics, graphene and 2D materials, as well as nanolaminates) were held at the IMDEA Materials Institute in 2013. These took full advantage of the facilities available in the new building. Over 400 researchers from 30 countries attended the events, enhancing the international visibility of our activities.

1. **Magnesium Workshop Madrid 2013, International Workshop on Processing-Microstructure-Mechanical Properties of Magnesium Alloys,** C. J. Boehlert, J. LLorca, M. T. Pérez-Prado (Conference Chairs), May 2013.

2. **TKM-2013, International Workshop on Materials Design Process: Thermodynamics, Kinetics and Microstructure Control**, J. M. Torralba, Y. Cui (Conference Chairs), June 2013

3. **International Workshop on Synthesis, Properties and Applications of Graphene and 2D Materials**, J. J. Vilatela (all conference chairs), July 2013

4. **Multilayers´13, International Workshop on the Mechanical Behaviour of Nanoscale Multilayers**, J. M. Molina-Aldareguia, I. Martín-Bragado, J. LLorca (Conference Chairs), October 2013

Figure 4. Conference facilities at IMDEA Materials Institute. Main hall during a poster session.

Figure 5. IMDEA Materials Institute Auditorium during an oral presentation.

6.5 Invited Seminars and Lectures

1. *"Plastic deformation at high temperature at nm and μm scale"*. J. LLorca, Faculty of Mechanical Engineering**, Technion Israel Institute of Technology**, Haifa, Israel, January 2013.

2. *"Persistent Organic Pollutants (POPs) and Environmentally Friendly Flame Retardant Materials"*. D. Y. Wang, **Shenyang University of Chemical Technology**, Shenyang, China, February 2013.

3. *"High temperature nanomechanics"*. J. LLorca, Department of Engineering Science, **Oxford University**, Oxford, UK, February 2013.

4. *"The challenge of technology transfer from academia: a success story in materials for aerospace"*. J. LLorca, **Airbus Military**, Getafe, Spain, February 2013.

5. *"Persistent Organic Pollutants (POPs) and Environmentally Friendly Flame Retardant Materials"*. D. Y. Wang, **Chongqing University of Arts and Sciences**, Chongqing, China, March 2013.

6. *"Development of Fire Retardant Polymer Nanocomposites"*. D. Y. Wang, Institute of Chemistry, **Chinese Academy of Sciences**, Beijing, China, March 2013.

7. *"Development of Fire Retardant Polymer Nanocomposites"*. D. Y. Wang, **Beijing Institute of Fashion Technology**, Beijing, China, March 2013.

8. *"Plasticity of lightweight Mg alloys at the macro and micro scales"*. M. T. Pérez-Prado, **École Polytechnique Fédérale de Lausanne**, Lausanne, Switzerland, March 20 *"Desde las partículas hasta aleaciones y compuestos de matriz metálica de altas prestaciones"*, J. M. Torralba, Departamento de Ciencia de Materiales e Ingeniería Metalúrgica, **Universidad de Barcelona**, Barcelona, Spain, April 2013.

9. *"Nanocomposites of CNT and graphene"*. J. J. Vilatela, **University of Münster**, Münster, Germany, May 2013.

10. "*Nanocomposites: an effective way to imparting fire retardancy on polymeric materials"*. D. Y. Wang, **Hubei University**, Hubei, China, June 2013.

11. *"Nanocomposites: an effective way to imparting fire retardancy on polymeric materials"*. D. Y. Wang, **Wuhan textile University**, Wuhan, China, June 2013.

12. *"High temperature mechanical behavior of Nanoscale Multilayers"*. M. Monclús, **Centro de Tecnologías Físicas, CSIC**, Madrid, Spain, June, 2013.

13. *"Computational and experimental micromechanics of composites. A mature discipline?"*. C. González, J. LLorca, Department of Aerospace Engineering, **University of Bristol**, Bristol, UK, June 2013.

14. *"Multiscale modelling of composites: a roadmap towards virtual testing"*. C. González, J. LLorca. Department of Aerospace Engineering, **University of Bristol**, Bristol, UK, June 2013.

15. *"Multiscale modelling of composites: a roadmap for virtual testing"*. J. LLorca, Department of Materials Science and Engineering, **Shanghai Jiaotong University**, Shanghai, China, June 2013.

16. *"High temperature nanomechanics"*. J. LLorca, Department of Materials Science and Engineering**, Shanghai Jiaotong University**, Shanghai, China, June 2013.

17. *"On the quest of engineering ceramics for very high temperature structural applications"*. J. LLorca, Department of Materials Science and Engineering, **Shanghai Jiaotong University,** Shanghai, China, June 2013.

18. *"Multiscale Engineering of Carbon Nanotube fibres"*. J. J. Vilatela, **IMDEA Nanoscience Institute**, Madrid, Spain, July 2013.

19. *"Multiscale modelling of composites: a roadmap for virtual testing"*. J. LLorca, Energy Research Institute, **Nanyang Technological University**, Singapore, July 2013.

20. *"High temperature nanomechanics"*. J. LLorca. Department of Materials Engineering, **Indian Institute of Science**, Bangalore, India, August 2013.

21. *"Multiscale modelling of composites: a roadmap for virtual testing"*. J. LLorca, Department of Materials Engineering, **Indian Institute of Science**, Bangalore, India, August 2013.

22. *"Nanomaterials for energy"*. J. J. Vilatela, **Repsol Research Centre**, Madrid, Spain, September 2013.

23. *"New Ideas on Fire Retardancy of Polymeric Materials"*. D. Y. Wang, **Leibniz Institute of Polymer Research Dresden**, Dresden, Germany, October 2013.

24. *"New High Performance Polymeric Materials"*. D. Y. Wang, **Fraunhofer Institute for Structural Durability and System Reliability**, Darmstadt, Germany, October 2013.

25. *"Simulation of plastic behavior at different length scales: from the nano to the macro-scale"*. J. Segurado, **Universita degli studi di Brescia**, Brescia, Italy, October 2013

26. *"High temperature nanomechanics"*. J. LLorca, Department of Mechanical Engineering, **National University of Singapore**, Singapore, October 2013.

27. *"Instituto IMDEA Materiales de la Comunidad de Madrid: una experiencia innovadora basada en el liderazgo y la atracción de talento*ω J. M. Torralba, **Tecnológico de Monterey,** Monterrey, México, November 2013.

28. *"High temperature nanomechanics"*. J. LLorca, Laboratoire de Mécanique et Technologie, **l'Ecole Nationale Supérieure de Cachan**, Cachan, France, November 2013.

29. *"Kinetic Monte Carlo simulation for technological processes"*. I. Martin-Bragado, **Universidad Complutense**, Madrid, Spain, November 2013.

30. *"Kinetic Monte Carlo simulation for technological processes"*. I. Martin-Bragado, **Universidad Católica de Murcia**, Murcia, Spain, December 2013.

6.6 Seminars

1. *"Modelling and simulation of damage by nucleation and void growth: a multiscale approach"*, **Dr. Celia Renia** (from Lawrence Livermore National Laboratory, Livermore, California, USA). January 2013.

2. *"In situ nanomechanics at elevated temperature and its application to crystalline materials"*, **Dr. Jeffrey Wheeler** (from EMPA, The Swiss Federal Laboratory for Materials Science and Technology, Thun, Switzerland). February 2013.

3. *"Ceramic-metal nanocomposites"*, **Prof. José Serafín Moya** (from ICMM-CSIC, Instituto de Ciencia de Materiales de Madrid, Madrid, Spain). February 2012.

4. *"Hybrid systems based on semiconductor nanocrystals"*, **Dr. Beatriz Hernández** (from IMDEA Nanoscience Institute, Madrid, Spain). June 2013.

5. *"Charge, phonon and spin transport in complex forms of structurally and chemically modified forms of graphene materials"*, **Prof. Stephan Roche** (from Institut Català de Nanociència i Nanotecnologia, Barcelona, Spain). July 2013

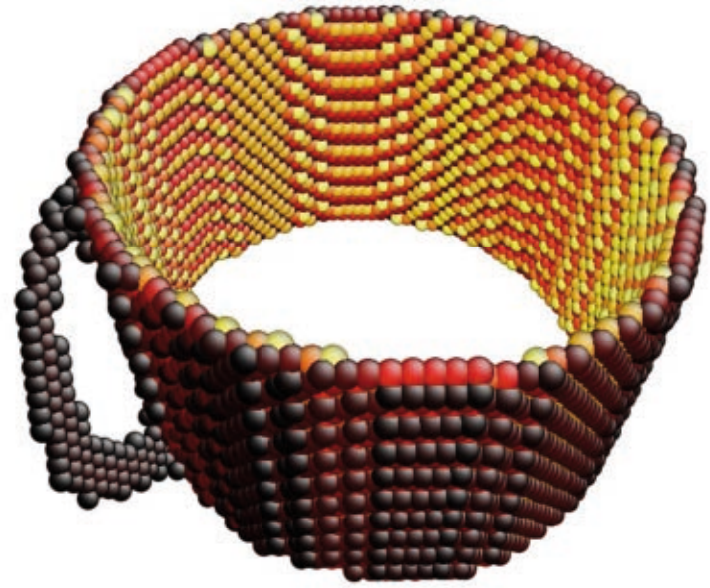
6. *"Study on properties of Eucommia ulmoides gum toughening Plastics"*, **Prof. Qinghong Fang** (from School of Materials Science and Engineering, Shenyang University of Chemical Technology (SUCT), Shenyang, China). July 2013.

7. *"Computational discovery of materials for clean and energy efficient technologies"*, **Dr. Maciej Haranczyck** (from Lawrence Berkeley National Laboratory, Computational Research Division, Berkeley, California, USA). September 2013.

8. *"Development of sustainable polymer materials and composites"*, **Dr. Xiaoqing Zhang** (from CSIRO Materials Science and Engineering, Australia). September 2013.

9. *"Magnetic devices"*, **Dr. Lucas Pérez** (from Complutense University of Madrid, Madrid, Spain). November 2013

seminars



fellowships

6.7 Fellowships

1. *Amarout Programme, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme*

- Call 2013: **Dr. D. Y. Wang, Dr. D. W. Lee, Dr. J. Wan, Dr. B. Gan, Dr. B. Tang, Dr. X. Wang**
- 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. Jerusalem**

2. *Ramon y Cajal Programme, Spanish Ministry of Economy and Competitiveness*

- Call 2012: **Dr. I. Martin-Bragado, Dr. D. Y. Wang**
- Call 2011: **Dr. R. Guzman de Villoria, Dr. I. Sabirov**
- Call 2010: **Dr. A. Dasari, Dr. S. Milenkovic**

3. *Juan de la Cierva Programme, Spanish Ministry of Economy and Competitiveness*

- Call 2012: **Dr. H.-J. Chang**
- Call 2011: **Dr. J. J. Vilatela, Dr. C. S. Lopes, Dr. S. R. Bonta**
- Call 2010: **Dr. R. Seltzer**
- Call 2009: **Dr. A. Jerusalem**

4. *China Scholarship Council*

- Call 2013: **Y. Pang, Y. Lingwei**
- Call 2012: **Y. Chen, X. Zhao**
- Call 2011: **G. Xu, H. Yue**

5. *Cajal Blue Brain Project, Spanish Ministry of Economy and Competitiveness*

- **J. García**

6. *Training University Lecturers (FPU) Programme, Spanish Ministry of Education, Culture and Sport*

- Call 2012: **F. Martínez**

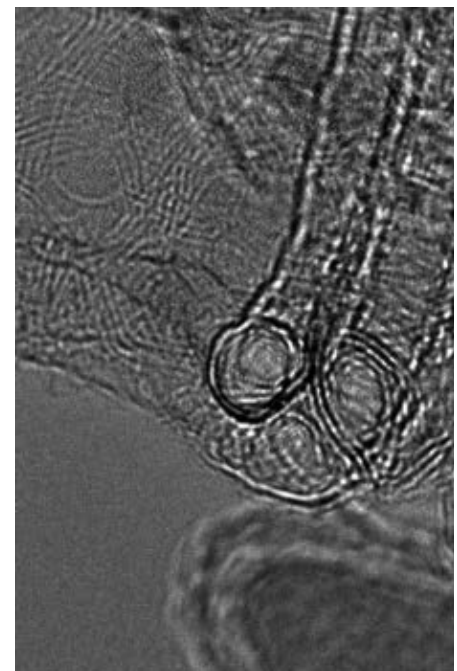
7. *Predoctoral Fellowships Programme, Spanish Ministry of Economy and Competitiveness*

- Call 2013: **A. Palomares**

6.8 Awards

- Shanghai Jiaotong University, Shanghai, China, Guest Professorship.
  Prof. J. LLorca
- Indian Institute of Science, Bangalore, India, Brahm Prakash Visiting Professorship.
  Prof. J. LLorca
- Elected to the Academia Europaea, Physics and Engineering Section.
  Prof. J. LLorca
- Distinguished Service Award 2013, European Powder Metallurgy Association.
  Prof. J. M. Torralba
- 2013 IUMA Young Researchers Award, Institute of Materials, University of Alicante.
  Dr. J. J. Vilatela
- Shenyang University of Chemical Technology, Shenyang, China, Guest Professorship.
  Dr. D. Y. Wang

awards



6.9 Institutional Activities

- Member of the *European Composites, Plastics and Polymer Processing Platform* (ECP4)
- Local Contact Point of the EURAXESS pan-European initiative
- Member of the Steering Committee of the *Spanish Technological Platform of Advanced Materials and Nanomaterials* (MATERPLAT)
- Member of the Technological Clusters on Security and Renewable Energies promoted by *Madrid Network*.
- Member of the Network of Research Laboratories of *Comunidad de Madrid* (REDLAB)
- Co-organizers of the *Interuniversity Research Seminars Programme* (hosting to J. W. Hutchinson, Harvard University and G. Holzapfel, University of Graz)
- Participation in the "*XIII Semana de la Ciencia"*, promoted by *Madri+d*
- Participation in the "*Noche de los investigadores"*, promoted by *Fundación Madri+d*

institutional activities

6.10 Theses

6.10.1 PhD Theses

"Cure, Defects and Mechanical Performance of Fiber-Reinforced Composites"
Student: Silvia Hernández
Technical University of Madrid
Advisors: Prof. J. LLorca and Dr. C. González
Date: March 2013.

6.10.2 Master/Bachelor Theses

"Fatigue Damage Sensing and Electrical Monitoring of Carbon Nanotube Composites"
Student: Anna Sorribes
Technical University of Madrid
Advisor: Dr. J. J. Vilatela
Date: February 2013

"LDH-based Epoxy Nanocomposites"
Student: José Ignacio Núñez Peñas
Technical University of Madrid
Advisor: Dr. D. Y. Wang
Date: June 2013

"Fire Retardant Epoxy and Its Properties"
Student. Héctor Merchán Bustero
Technical University of Madrid
Advisor: Dr. D. Y. Wang
Date: June 2013

"CNT fibres for structural health monitoring in ceramic composites"
Student: Alfonso Monreal
Technical University of Madrid
Advisor: Dr. J. J. Vilatela
Date: June 2013

"Thermoplastic Interleaves for carbon fiber composite materials"
Student: Hugo Mora
Technical University of Madrid
Advisor: Dr. R. Guzmán de Villoria
Date: June 2013

"Hybrid Mechanical Thermal Barriers for Aerospace Composite Laminates"
Student: Juan Carlos Toribio
Technical University of Madrid
Advisor: Dr. R. Guzmán de Villoria
Date: June 2013

"Numerical study of polimeric material HST in morphing structures"
Student: Santiago García Rodriguez
Technical University of Madrid
Advisor: Dr. J. Segurado
Date: July 2013

"Measuring the CRSSs of Magnesium and its alloys by instrumented nanoindentation"
Student: Raúl Sánchez
Carlos III University of Madrid
Advisors: Dr. J. M. Molina-Aldareguia and Dr. M. T. Pérez-Prado
Date: July 2013

"Deformation behavior of a high strength multiphase steel created via the quenching and partitioning process at macro- and microscales"
Student: Irene de Diego
Carlos III University of Madrid
Advisors: Dr. I. Sabirov and Dr. J. M. Molina-Aldareguia
Date: July 2013

"Synthesis and properties of CNT fibres and their composites"
Student: Bartolomé Mas
Carlos III University of Madrid
Advisor: Dr. J. J. Vilatela
Date: September 2013

"Vertically aligned nanotubes synthesized on stainless steel"
Student: Pablo Romero
Carlos III University of Madrid
Advisor: Dr. R. Guzmán de Villoria
Date: September 2013

"Hybrid nano-architectures based on carbon nanotubes and nanoparticles"
Student: Luis Carlos Herrera
Carlos III University of Madrid
Advisor: Dr. R. Guzmán de Villoria
Date: September 2013

"Experimental, analytical and numerical investigation of loading rate effects on mode I, mode II and mixed mode I-II delamination in advanced CFRP"
Student: Luca di Stasio
Technical University of Milan
Advisors: Dr. C. S. Lopes and Dr. Alessandro Airoldi
Date: October 2013

"Self-healing of elastomer composites through click-chemistry"
Student: Diana Beneito
Technical University of Madrid
Advisors: H. Yue, Dr. J. P. Fernández-Blázquez and Dr. J. J. Vilatela
Date: October 2013

"Thermal conductivity of advanced materials"
Student: Ivan López
Technical University of Madrid
Advisors: Dr. I. Sabirov and Dr. J. J. Vilatela
Date: October 2013

"Synthesis and characterization of ordered B2-NiAl intermetallic by mechanical alloying",
Student: Arcadio Varona
Carlos III University of Madrid
Advisor: Dr. S. Milenkovic
Date: October 2013

theses

6.11 Internships / Visiting Students

"Synthesis and Modification of Nanomaterials"
Student: Hugo Drelon
Date: May-July 2013
Advisor: Dr. D. Y. Wang,
Visiting student from ENSAIT Chimie Lille, France

"Functionalized Nanomaterials and Bio-based Epoxy composites"
Student. Cheng Li
Date: March-September 2013
Advisor: Dr. D. Y. Wang
Visiting student from Leibniz Institute of Polymer Research Dresden, Germany

"Physical simulation of HAZ in welding"
Student: Daniel Fernando Atehortua
Date: June-October 2013
Advisor: Dr. I. Sabirov
Visiting student from University of Cali, Colombia

"Creep of solder alloys at the microscale"
Student: Carl Mayer
Date: July-August 2013
Advisor: Dr. J. M. Molina-Aldareguia
Visiting Student from Arizona State University

"Hot deformation and workability of Fe-Al-Nb alloys"
Student: Wenjing Li
Date: March-August 2013
Advisor: Dr. S. Milenkovic
Visiting student from Beijing University of Aeronautics and Astronautics

"Analysis of the microstructure and mechanical behaviour of a Mg-Mn-Nd alloy"
Student: Lisa Blanchard
Date: July-September 2013
Advisor: Dr. P. Hidalgo-Manrique
Visiting student from École Nationale Supérieure de Physique, Electronique, Materiaux de l'Institut Polytechnique de Grenoble

"Nanocomposites"
Student: Juan Larrea
Date: July-August 2013
Advisor: Dr. R. Guzmán de Villoria
Visiting student from Imperial College of London

"Study of interdiffusion on metallic materials"
Student: Hongjie Tang
Date: June-August 2013
Advisor: Dr. Y. Cui
Visiting student from Michigan State University, USA

6.12 Courses

"Non conventional composites"
Master in Composite Materials
Technical University of Madrid and EADS
Professors: Dr. J. J. Vilatela, Dr. R. G. de Villoria, Dr. I. Sabirov and Prof. J. Llorca

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

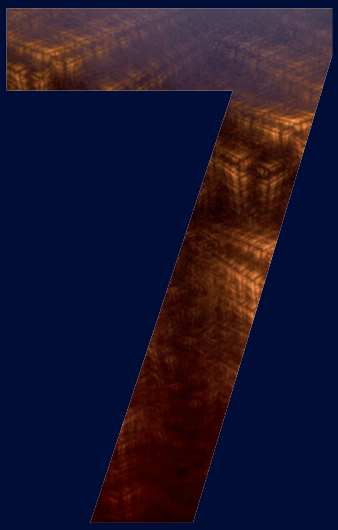
"Mechanics of composite materials"
Master/ Doctoral Program in Engineering of Structures, Foundations and Materials
Technical University of Madrid
Professors: Dr. J. Segurado and Dr. C. González

"Simulation in materials engineering"
Master/ Doctoral Program in Materials Engineering
Technical University of Madrid
Professors: Prof. J. LLorca, Dr. C. González, Dr. C. S. Lopes, Dr. I. Martin-Bragado and Dr. Y. Cui

"Impact Behavior of Materials"
Master/ Doctoral Program in Materials Engineering
Technical University of Madrid
Professor: Dr. C. S. Lopes

"Non-equilibrium processes in materials and nanophysics"
Master in Nanophysics and Advanced Materials
Complutense University of Madrid
Professor: Dr. I. Martin-Bragado

scientific highlights



annual report 2013

monte carlo

Monte Carlo simulation of epitaxial structures for microelectronic devices

of epitaxial structures for microelectronic devices

Tools for novel microelectronics

Advances in the processing of microelectronic devices are significantly fast in both the incorporation of technologies and integration of new materials. In particular, old 2D-like complementary metal-oxide-semiconductor (CMOS) technologies are discarded in favour of modern 3D topologies, with good examples being the massive use of finFETs in production lines and the trend to incorporate vertical integration in improving device connectivity. For materials, although silicon remains (and will do so for some time) the workhorse of the microelectronics industry, new candidates are emerging in a complex scenario. Si-like materials, in particular Ge and Si-Ge, are gaining interest while III-V materials (such as InGaAs), also invite research. These new materials benefit from higher charge carrier mobilities, allowing the development of even faster technologies.

The introduction of novel 3D topologies and new materials is very much dependent on the research of epitaxial growth of semiconductors. Solid phase epitaxial regrowth (SPER), i.e., the recrystallisation of an amorphous phase in contact with a crystalline one, is used to both heal the device after doping and increase the activation of such dopants. In addition, novel 3D topologies are partly built by epitaxial growth. Consequently, the modelling of this phenomenon is a field of large interest for the microelectronics industry in replacing costly experiments. For this reason, the IMDEA Materials Institute has developed an atomistic lattice kinetic Monte Carlo tool (as a module of the general Monte Carlo Simulator MMonCa [1]) that accurately simulates epitaxial processes. Kinetic Monte Carlo has been chosen because it accounts for realistic processing times (something that was not possible with molecular dynamics) while providing atomistic detail, a feature of critical importance in epitaxy that is lost when using continuum methods.

Examples of application of this new tool include the bimodal growth of Si(111) by SPER[2] and the effects of stress during epitaxial growth on Si(100) [3]. The importance of correctly including the formation of twins during epitaxy to form defects, how these twins create distinct defective areas depending on the initial orientation, and how stress affects the overall growth of the crystal, and also the production of defects, have been demonstrated. Figure 1 and Figure 2 show the strong influence of defects on the morpho logy of distinct surfaces, and how the creation of tilted twins dramatically changes the recrystallisation process. Finally, such a technique was extended to other materials by

adapting our model to simulate Ge SPER [4], with research continuing on the epitaxial processing of SiGe and III-V materials looking into the near future.

References

[1] I. Martin-Bragado *et al. "MMonCa: an object Kinetic Monte Carlo simulator for damage irradiation evolution and defect diffusion"*, **Computer Physics Communications 184**, 2703–2710, 2013.

[2] 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, 2012.

[3] B. Sklenard *et al. "An atomistic investigation of the impact of in-plane uniaxial stress during solid phase epitaxial regrowth"*, **Applied Physis Letters 102**, 151907, 2013.

[4] B. L. Darby *et al*. "*Substrate orientation dependence on the solid phase epitaxial growth rate of Ge"*, **Journal of Applied Physics 113**, 033505, 2013.

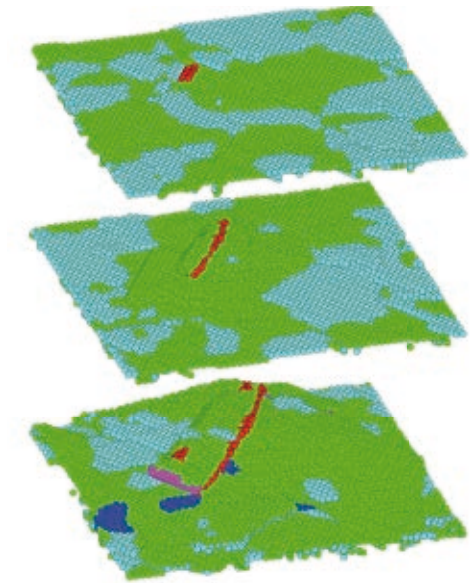


Figure 1. Evolution of an amorphous/crystalline Si(111) interface at 550º C. The green atoms are grown in the substrate orientation. All the other atoms are twin nano-crystals. In particular, the blue atoms are compatible with the planar original front, but the red atoms produce an inclined twin that drastically changes the topology of the regrown front.

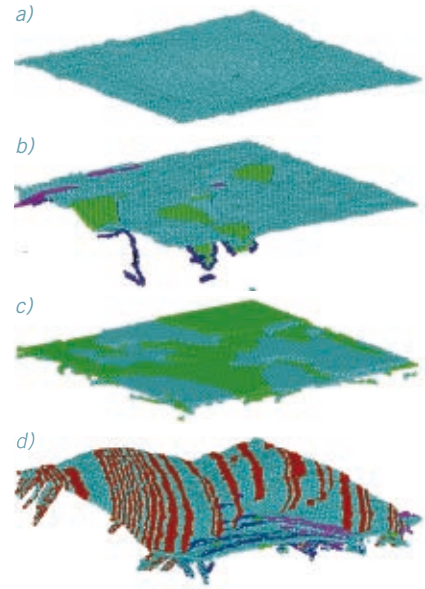


Figure 2. Morphologies for different Si recrystallized orientations, as simulated with MMonCa. a) the Si(100) amorphous/crystalline interface is the most perfect one, while for b) Si(110) some defects appear that increase the surface roughness. c) Si(111) advances forming very planar twin crystals competing with the regular ones at the beginning, but d) the formation of inclined twins provides the seed for an irregular structure.

understanding

Understanding resin microflow by X-ray computed tomography

by X-ray computed tomography

Processing of high performance composite materials

Fiber-reinforced polymers are extensively used in structural components for engineering applications. At the time of writing, high performance composites have to be manufactured in autoclave to ensure that they are pore free which has led to high processing costs and subsequent large interest in the optimization of out-of-autoclave processing techniques. Vacuum assisted resin transfer moulding (VARTM) is a significantly appealing process due to its relative low cost and possibility of processing large panels. In this process, the liquid resin is infiltrated into a plastic bag that contains the fibre preform that lies on a rigid mould. Infiltration is assisted by the application of vacuum. However, the resin flow through the fiber fabric is highly complex and the key parameters that control the nucleation, growth and coalescence of pores during infusion are not well understood. In addition, the resin flow in the fabric takes place at two different length scales: macroscopic resin flow between the fiber tows progresses rapidly, while microflow within the fiber tows occurs at lower speed [1, 2]. The interaction between macroflow and microflow is known to be a critical factor in controlling the development of porosity, though it is difficult to analyse it experimentally.

In order to provide the experimental evidence necessary to understand resin flow during VARTM, the researchers of IMDEA Materials Institute have developed a miniaturised device that reproduces the conditions of the VARTM process and, at the same time, allows study of the infiltration at both scales by means of synchrotron and laboratory X-ray computed tomography (XCT). To this end, high resolution synchrotron XCT was performed at the fibre scale to analyse in situ macro- and micro-flow behaviour and the defect formation during the infusion process. Figure 1 shows the experimental set-up at the P05 beamline at DESY Synchrotron in Hamburg where the experiments were performed. The liquid is infiltrated from the top (inlet) and the vacuum applied at the bottom (outlet). The fibre tow specimen, placed in a vacuum bag inside the polymethylmethacrylate (PMMA) tube was scanned by X-rays during infiltration.

Figure 2 shows a reconstructed volume and a cross-section obtained by synchrotron XCT, displaying the flow front (macroflow) around the tow and the microflow inside the tow.

resin microflow

This unique experimental set-up provides the information required to analyse the resin flow in 3-dimensions during infiltration at both the microscale and the macroscale, as well as to assess the differences in permeability between both regimes, with the former being several orders of magnitude lower than the latter. Moreover, the experiments show the conditions that give rise to regions that might remain partially infiltrated due to trapped air bubbles or differences between capillarity and resin pressure, leading to low quality panels. Based on these data, it is possible to design optimised VARTM strategies to improve the quality and reduce the processing cost of advanced structural composites.

References

[1] J. M. Lawrence *et al. "Modeling the impact of capillary pressure and air entrapment on fiber tow saturation during resin infusion in LCM"*, **Composites: Part A 40**, 1053-1064, 2009.

[2] V. Neacsu *et al. "Use of magnetic resonance imaging to visualize impregnation across aligned cylinders due to capillary forces"*, **Experiments in Fluids 42**, 425–440, 2007.

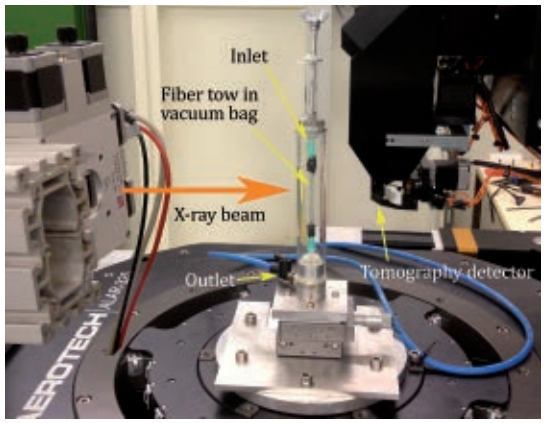


Figure 1. Experimental set-up prepared to study in situ the infiltration process at the P05 beamline of DESY Synchrotron.

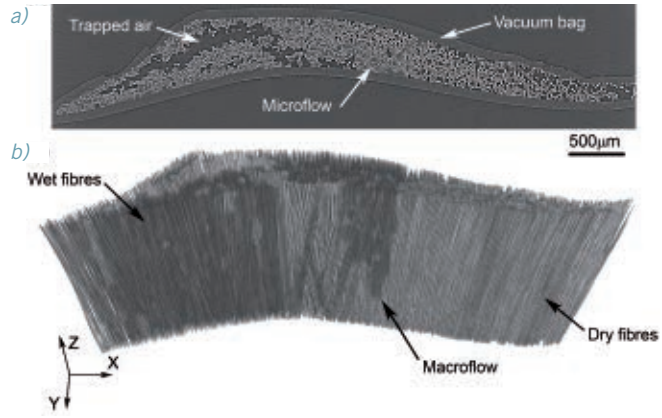


Figure 2. (a) Cross section of the scanned fibre tow specimen in the vacuum bag. Wet glass fibres are surrounded by the lighter grey colour. (a) 3D reconstruction of the infiltrated tow.

electrical curin

Electrical curing of adhesive thermosets by using nanotubes

thermosets by using nanotubes

E-CURE: alternative to conventional oven curing of thermosetting polymers

Adhesive bonding is of primary importance for the manufacture of structural components in the aerospace industry. There are multiple structural bonded joints in a modern aircraft throughout the wings and fuselage. Bonded patches are also used to repair composite panels, cracks in metallic parts or as reinforcement of deficient structures. IMDEA Materials Institute and Airbus Operations have worked together in exploring the use of novel conductive adhesives that can reduce fabrication and repair times.

The IMDEA Materials Institute has developed conductive epoxy resins that can be cured through resistive heating simply by passing an electric current through them [1, 2]. Electrical conductivity is obtained by the dispersion of carbon nanotubes (CNT) or graphene in the epoxy, which form a conductive network even at extremely low mass fractions (<0.5%). The process is intrinsically efficient, since heat is generated directly from within the sample and because the small distance between nanotubes (<100nm) results in exceptionally fast heating rates (up to 740°C/min). In addition, it is applicable to virtually any thermoset and any high-aspect ratio conductive nano filler.

The electrically curable thermosets are prepared by adding a known weight of nanotubes (or graphene) to the epoxy resin, which are dispersed by calendering using a three-roll mill (see Figure 1). Processing parameters such as mass fraction, calendering speed and resin temperature require adjustment to control the final conductivity of the thermoset according to the particular curing conditions of the application.

In the context of aerospace materials, the potential of these thermosets lies in the possibility of joining two conductive parts (either metallic or composite) faster and using less energy than in traditional methods. The process for bonding the two parts is achieved through using a PID controller, which continuously monitors the temperature (by means of an infrared camera, a pyrometer or thermocouples) to adjust the electric power delivered to the sample to follow a predetermined curing cycle (Figure 2). Robust adhesive joints can be produced by using either direct current (DC) or alternating current (AC).

The mechanical properties of electrically cured bonded joints show results that are comparable to those obtained by traditional oven curing. Single-lap shear strengths of carbon-fibre reinforced polymers parts cured electrically are currently within 80% of those cured in an oven, though they requiring roughly a quarter of the energy to cure.

g of adhesive

The next stage of the joint work carried out by IMDEA Materials Institute and Airbus Operations is directed at improving the curing process to match mechanical properties of oven-cured samples. This will be achieved by reducing porosity, increasing temperature uniformity and stabilising the conductivity of the thermoset at high temperatures. We anticipate this work to be of technological interest in other industrial sectors, such as the automotive and oil and gas, and to contribute to improving our understanding of the rheology of nanoparticle/polymer systems.

Acknowledgements

This project was partially funded by the Airbus Incubator Programme. Technical support from J. C. Rubalcaba on the design/fabrication of the curing control system is gratefully acknowledged.

References

[1] B. Mas *et al. "Thermoset curing through Joule heating of nanocarbons for composite manufacture, repair and soldering"* **Carbon 63**, 523–529, 2013.

[2] J. J. Vilatela *et al. "Thermoset curing through resistive heating of nanocarbons".* **Patent Application** *PCT/EP2013/055659 (19 March 2013).*

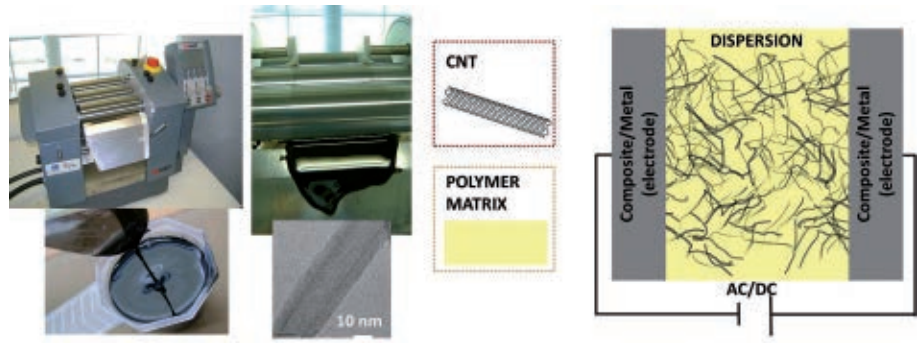


Figure 1. Photographs of the CNT/thermoset during calendering, TEM micrograph of a multiwalled CNT, and schematic of the method to join two conductive parts by resistive heating of a conductive CNT/thermoset adhesive.

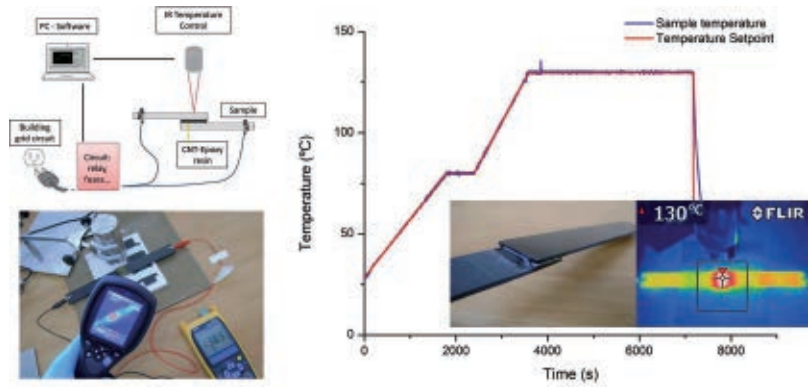


Figure 2. Schematic and photograph of the set-up used to join two carbon fibre composite parts and a plot of the sample temperature and set point during the process.

3d charaterisat

in Mg alloys

3D characterisation of twinning in Mg alloys

Seeing through metals

The density of Mg is one third that of aluminium and five times smaller than that of iron. Novel Mg alloys have a large potential to reduce the weight of vehicles for transportation. The worldwide effort toward reduced energy consumption has driven research activities to improve and optimise the strength and creep resistance of Mg, the lightest of all structural metals. This process requires support from a detailed knowledge of the critical deformation mechanisms that dictate the behaviour of Mg alloys.

Recent progress in the development of 3D characterisation techniques is leading to a more comprehensive understanding of the relationship between the microstructure and the properties of engineering materials. 3D electron backscatter diffraction (3D-EBSD), combining 2D EBSD software with the milling capabilities of a focused ion beam (FIB) and a field-emission gun scanning electron microscope (FEG-SEM), provides a three-dimensional characterisation of the morphology and orientations of individual grains, as well as a full description of grain boundaries (misorientation and boundary plane). This information is fundamental in recognising the microstructural factors that control twinning, one of the main deformation mechanisms of Mg alloys.

Together with dislocation slip and grain boundary sliding (at high temperature), twinning is the third process that contributes to the plastic deformation of Mg alloys. There remains much uncertainty as regards the influence of microstructural factors (grain size and orientation, among others) on the nucleation and growth of twins in Mg and, in particular, the interaction between twins and grain boundaries. Researchers at the IMDEA Materials Institute, in collaboration with the Max Planck Institute for Metals Research in Düsseldorf and the University of Oxford, have developed a multidisciplinary approach, based on 3D-EBSD and continuum mechanics modelling, to understand the effect of grain boundary misorientation (q) of twin propagation in AZ31 Mg alloy (Mg-3%Al-1%Zn) [1]. Figure 1 illustrates the analysed volume, consisting of a central grain that is favourably oriented to tensile twinning (P1), surrounded by boundaries of distinct misorientation angles. Tij denote the various active twin variants. Twin propagation becomes increasingly more difficult as q increases and high local stresses develop in the vicinity of grain boundaries, leading to local plasticity that is not directly related to the applied stress. Furthermore, the 3D morphology of individual twin variants has been associated with their orientation with respect to the applied stress, given

ion of twinning

by the Schmid factor. High Schmid factor variants have well established plate morphology, while low Schmid factor variants adopt irregular shapes (Figure 2).

References

[1] A. Fernández *et al. "Three-dimensional investigation of the grain boundary-twin interactions in a Mg AZ31 alloy by electron backscatter diffraction and continuum modeling".* **Acta Materialia 61**, 7679-7692, 2013

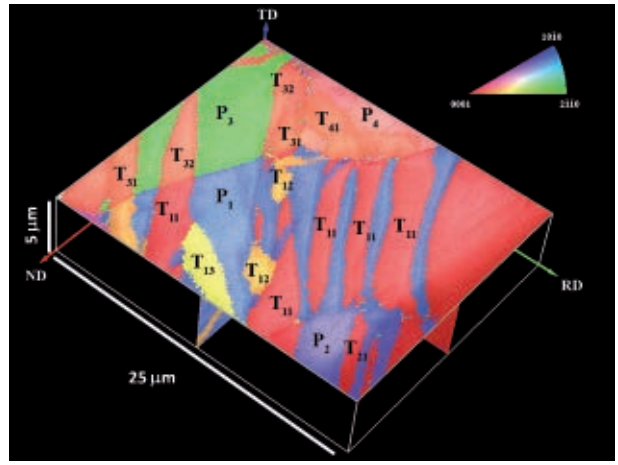
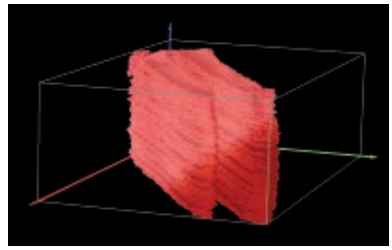


Figure 1. Volume analysed by 3D-EBSD. The orientation colour coding is included as an inset.

a)



b)

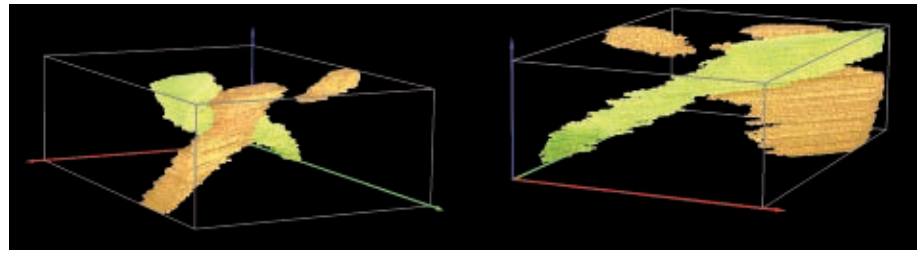


Figure 2. 3D morphology of different twin variants: (a) high Schmid factor; (b) low Schmid factor.

modelling for

Modelling for better castings

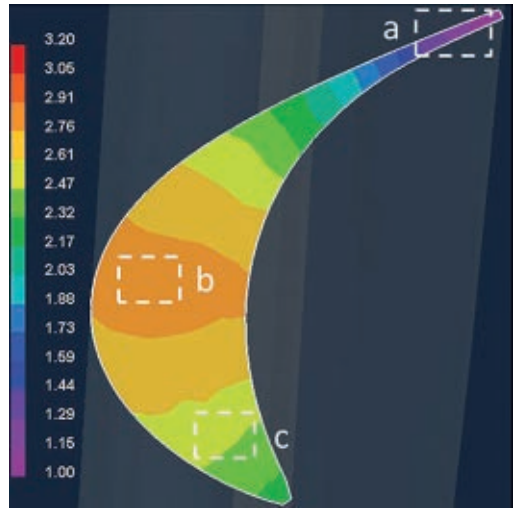
Predicting porosity and grain structure

Nozzle guide vanes (NGVs) are structural parts of gas turbines manufactured from Ni-based superalloys via investment casting. The search for reduced weight and increased efficiency of gas turbines is driving changes in NGV design towards more complex shapes and thinner geometries. However, these innovations are hindered by the complexity of investment casting of parts with extremely thin elements. The traditional route to optimising the investment casting of these complex parts entails a 'trial and error' approach or, in other words, experimental casting trials: the casting parameters are systematically varied until castings with acceptable porosity and grain structure are obtained. Obviously, given that this strategy is expensive and time consuming it significantly limits the rate of innovation. In order to overcome these limitations, six partners joined the VANCAST project (named, the "Next Generation Nozzle Guide Vanes") to develop a novel modelling tool capable of predicting porosity and grain structure in the as-cast NGVs.

The new simulation tool consists of three modules designed to predict the thermal history, porosity and grain structure. The thermal module accurately describes the thermal history at each point of the cast during solidification/cooling and provides input information for the other modules. The ProCAST-based model for porosity determines the hot spots and areas with enhanced porosity that develop in localised regions of the cast during solidification. Finally, the cellular automata and finite element (CAFE) module provides information about the local grain structure (grain size and shape) throughout the cast. All three modules were validated against experimental casting trials. Figure 1 illustrates the accuracy of the model prediction for porosity in a transversal section of a solid vane, while the experimental grain structure of the hollow vane showed sound agreement with the model results, Figure 2. The new modelling tool can be used to carry out "virtual casting trials" and obtain, by means of simulations, the optimum parameters for investment casting. This will lead to a spectacular reduction in the number of experimental casting trials and will enhance the rate of innovation to develop more efficient NGVs.

The VANCAST project was funded by the European Union (EU) under the ERA-NET MATERA+ scheme of the 7th Framework Programme. The project was coordinated by the IMDEA Materials Institute and included the Swiss University of Applied Sciences and four industrial partners: an NGV designer (Industria de Turbo Propulsores), two investment casting companies (Precicast Bilbao and Precicast Novazzano) and a software company (Calcom-ESI).

better castings



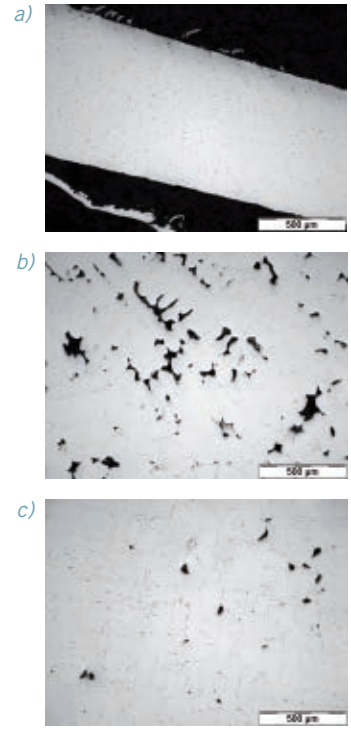


Figure 1. Porosity prediction by the modelling tool (left) and optical microscopy images of porosity in the indicated areas of the solid vane of the as-cast NGV (right). The location of the analysed section is marked by a red circle in the NGV icon (bottom left).

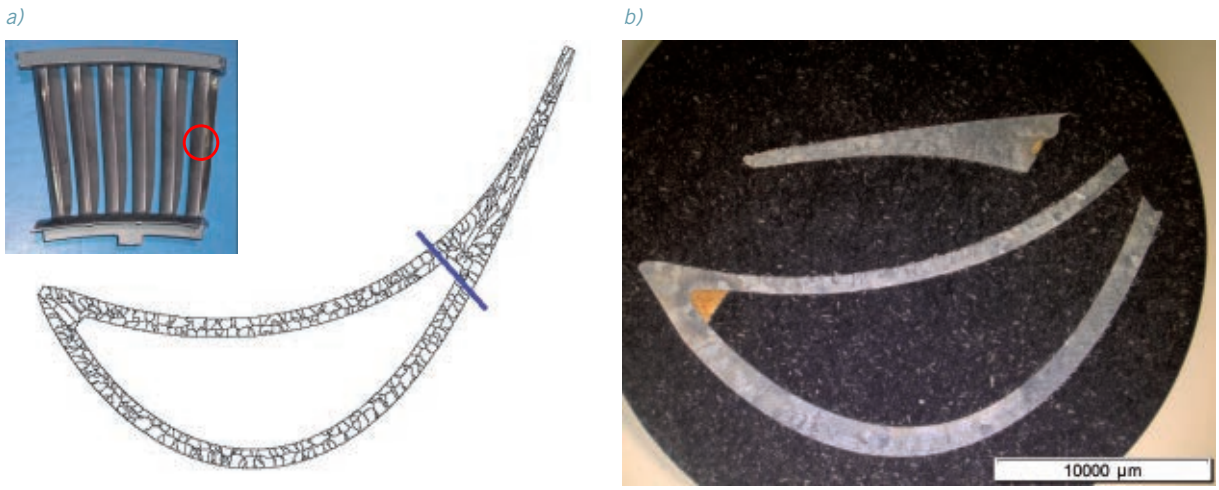


Figure 2. Grain structure predicted by the modelling tool (a) and optical microscopy image of the grain structure in the solid vane of the NGV (b). The dashed line on (a) marks the cut plane on (b). The location of the analysed section is marked by the red circle on the NGV icon (a).

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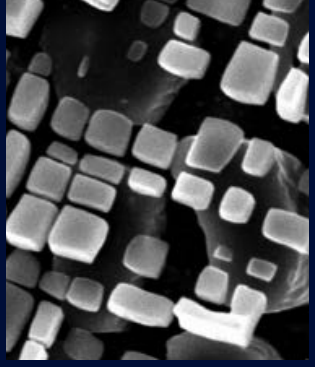

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