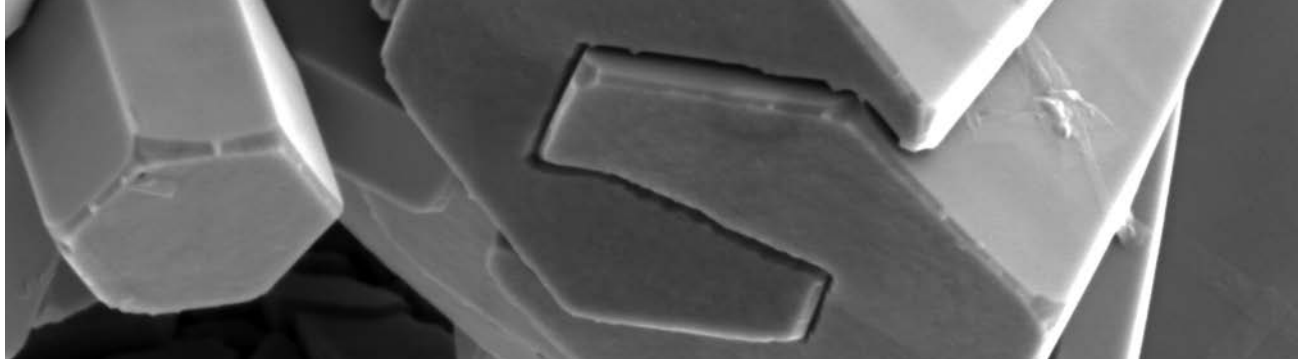

imdea materials institute

excellence as our technological key

institute imdea materials

annual report 2014

foreword

foreword

Javier LLorca
Director, IMDEA Materials Institute
March 2015

annual report
2014

Nobody doubts that the ability to attract talent is the key to success in any academic institution. And this is so for various reasons, of which not all of them are obvious. Because talent is distributed throughout the world, internationalisation is a must if you want to reach "the best and the brightest" in your field. And when these bright individuals arrive at your organisation, they not only bring their knowledge but also their international network of colleagues who are more than willing to continue with the collaboration. And this opens the possibility for exploring uncharted territories.

During 2014, the IMDEA Materials Institute has reinforced its commitment to promoting technological leadership with nine new research contracts directly funded by industrial enterprises. While seven projects have entailed collaboration with companies established in Spain which have selected the Institute as one of their strategic partners in research, four projects have been signed with multinational companies from the Netherlands, United Kingdom, United States of America and Taiwan. These organisations were unable to find the talent they had sought elsewhere because it had moved to Madrid.

Another important event in 2014 has been the award of doctorates to 10 graduate students who carried out their research at the Institute. And I am happy to report that all have found new positions to continue their careers either in industry or in the most prestigious research institutions in Europe (École Polytechnique Fédérale de Lausanne, Imperial College, Max-Planck Institute, University of Cambridge, …). Moreover, three received awards to the best doctoral thesis granted by the respective universities.

While the activities of the Institute during 2014 are summarised in the pages that follow, it is worth noting that multidisciplinary expertise has been enhanced with the incorporation of two new staff researchers in the areas of computational solid mechanics and X-ray characterisation of materials. Furthermore, the research capabilities have been expanded with three universal mechanical testing machines for the characterisation of mechanical properties of bulk materials and fibres under static and fatigue loading, together with a drop weight tower to study the mechanical behaviour of materials under impact and an actuator for *in situ* mechanical testing within the scanning electron microscopes.

Research activities in the four research programmes have led to the publication of 81 articles in international peer-reviewed journals and one patent application, together with 42 plenary/keynote lectures at international conferences and 23 invited seminars at prestigious research institutions and universities throughout the world. In addition, the code MMonCa, an object kinetic Monte Carlo simulator for damage irradiation evolution and defect diffusion, developed by the Institute has been licensed to the Danish company QuantumWise and will be incorporated into the Atomistic Toolkit software suite dedicated to multi-scale modelling of material properties. These results – and many others included in the 2014 Annual Report – manifest the international standing of the research activities of the Institute and its commitment to expansion in such a direction.

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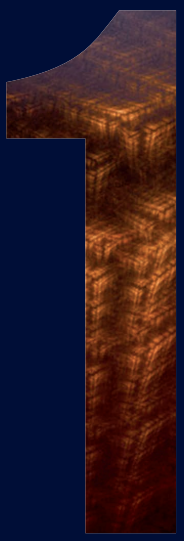


annual report 2014

1.1. About the IMDEA Materials Institute

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

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

1.2. Strategic industrial partnership

Collaboration with industry to promote technological leadership, together with research of excellence, has always been an essential part of the Institute's objectives. The initial research lines of the Institute were established by its Scientific Council after consultation with a number of companies which agreed to establish long-term partnerships. Companies benefited from the international and multidisciplinary talent concentrated in the Institute, as well as from the research infrastructures. In turn, they have committed themselves to developing one or several research lines in collaboration with IMDEA Materials Institute.

This model of collaboration, initially limited to a number of companies established in Spain (either multinational or Spanish), has been fully validated during the eight years since the founding of the Institute. This has led to a constant growth in the number of industrial contracts and collaborations with industry within the framework of collaborative research projects funded by the European Union (EU), Government of Spain and Regional Government of Madrid.

During 2014, the model of building strategic partnerships with industry has expanded beyond Spain. Of the nine industrial research projects started in 2014, four contracts have been signed with multinational companies that have come to Madrid in search of the talent that they could not find elsewhere. These companies are B/E Aerospace (USA), world leader in the design and fabrication of aircraft interiors, Hexcel (UK), one of the major suppliers of advanced polymer composites for aerospace applications, a semiconductor materials related company (Asia/Pacific), and Fokker (The Netherlands), a manufacturer of advanced composite components for aeronautics.

In addition, the strategic partnership with Spanish companies (such as Airbus, ITP, Airbus Defence & Space, Acciona, Tolsa, FerroAtlántica, and Abengoa Research) has been strengthened with new research contracts or the development of current projects. The current list of active industrial partners of the Institute is depicted in the map in Figure 1.

Figure 1. Active strategic industrial partnerships of IMDEA Materials Institute

1.3. Appointments to the Board of Trustees and Scientific Council

Dª Lorena Heras Sedano, General Director of Universities and Research of the Madrid Regional government replaced Dr. Rocío Albert López-Ibor as one of the permanent trustees from the Regional Government of Madrid.

Prof. Manuel Ocaña, Senior Scientist at the Materials Science Institute of Seville (CSIC), replaced Dr. Ángel Arteaga Iriarte, Director of the Eduardo Torroja Institute for Construction Science (CSIC), as trustee from universities and public research institutions.

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

1.4. Organizational chart

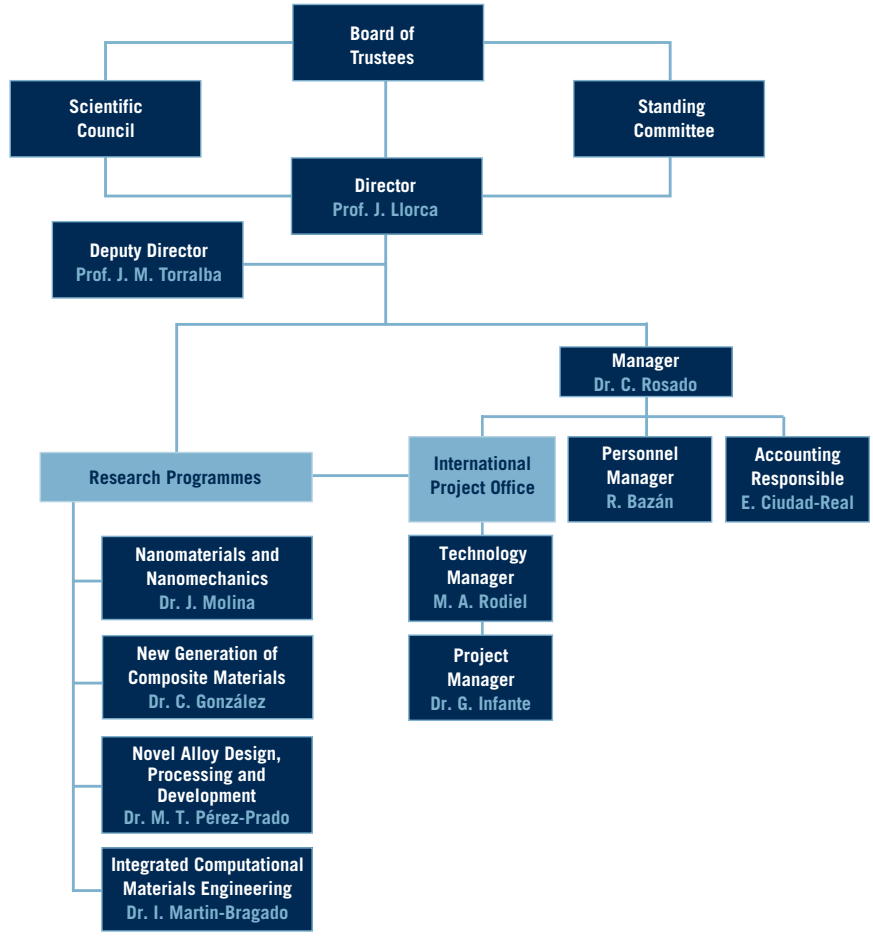


Figure 2. Organizational chart of IMDEA Materials Institute

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 Lorena Heras Sedano
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

Prof. Manuel Ocaña
Professor
Materials Science Institute of Seville (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
Professo
RWTH Aachen University, Germany

EXPERT TRUSTEES

Mr. Pedro Escudero
Managing Director
European Value Advisors

COMPANIES TRUSTEES

AIRBUS OPERATIONS S.L.
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

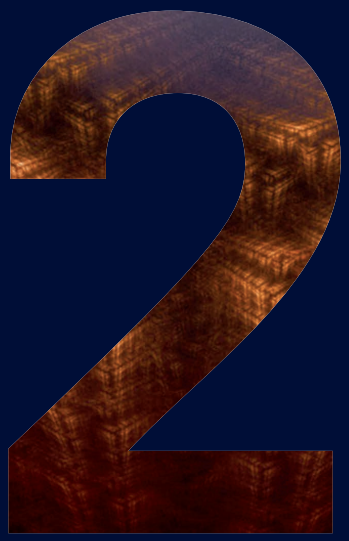
Prof. Eugenio Oñate
Director, International Centre for Numerical Methods in Engineering
Professor
Polytechnic University of Catalonia, Spain

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



annual report 2014

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 of them.

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.

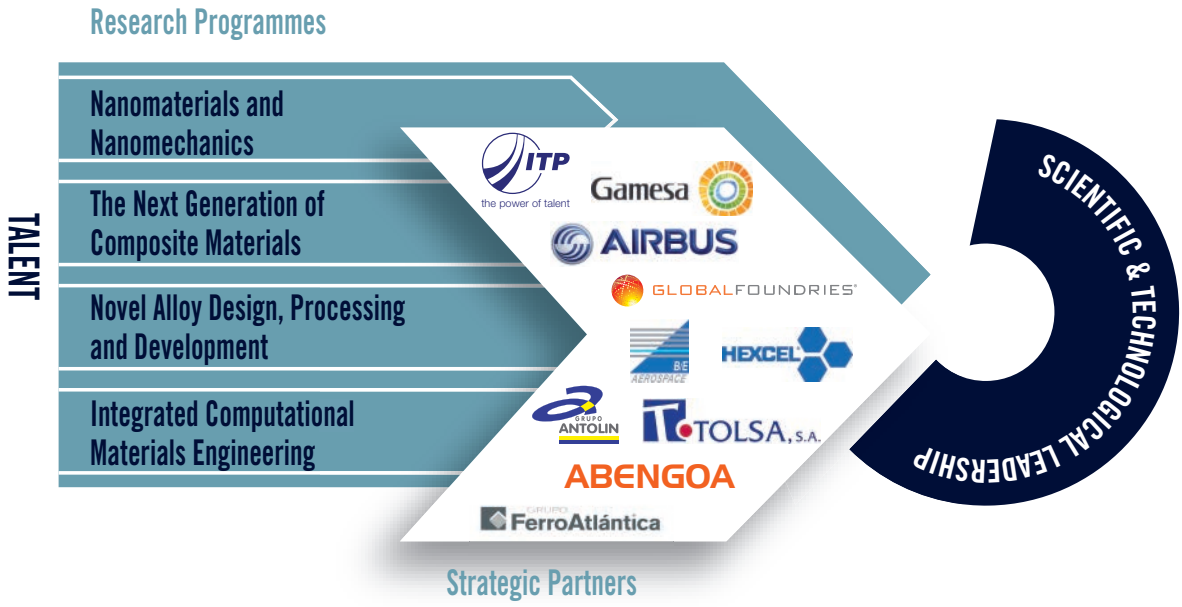


Figure 3. Research programmes and strategic partners of IMDEA Materials Institute

Nanomaterials and Nanomechanics

- **Synthesis, emerging properties and integration of carbon-based nanomaterials (graphene, nanotubes, nanofibers and hybrids):**
  - *Nanomaterials for energy generation and storage:* nanocarbon/semiconductor hybrids for photocatalysis, energy harvesting and capacitors.
  - *Sensors:* chemical, piezoresistive, piezoelectric.
  - *Hierarchical materials:* materials design from the nanoscale to the macroscale, nano-reinforced materials, composite materials with enhanced electrical and thermal conductivity.
  - *Size effects in the mechanical behavior of multifunctional materials:* strength of graphene, nanotubes, nanofibers, fibers and their interfaces.

- **Synthesis and properties of polymer-based multifunctional nanocomposites:**
  - *Sustainable materials:* bio-based nanocarriers, novel guest-host nanomaterials, nano-cross linker, functional dye sensitized solar cell, multifunctional polymer nanocomposites, etc.
  - *Fire retardant materials through nanodesign:* Multifunctional nanomaterials to increase fire retardancy: layered double hydroxide (LDH), sepiolite, molybdenum disulphide (MoS_2), nanocarbon, nano metal hydroxide, novel functional nanomaterials, nanocoatings, etc.

- **Design of nanoscale multilayers for extreme environments:** high temperature coatings, radiation resistant applications, etc.

- **Microstructure-property** relationships and development of physically based models in complex metallic alloys (Mg alloys, Ni superalloys, TiAl intermetallics, etc.), including:
  - *3D Characterization of materials,* including microstructural, chemical and crystallographic information and X-Ray microtomography.
  - *High temperature nanomechanics:* Measuring phase and interphase properties using high temperature nanoindentation and micropillar compression up to 700ºC, including *in situ* measurements.
  - *Multiscale simulation of the mechanical behavior:* molecular dynamics, dislocation dynamics, crystal plasticity, finite elements. Experimental micromechanical tests are used for validation and for bridging scales.
  - *In situ mechanical testing* of macroscopic samples within the scanning electron microscope and/or synchrotron.

B/E AEROSPACE

Thomas Swan
Chemical manufacturing since 1926

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Research groups involved:

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

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, toughened composites, non-conventional lay-up configuration, green composites, etc.
- **Composites with multifunctional capabilities:** fire resistance, electrical and thermal conductivity, energy management, barrier properties, non-destructive evaluation and health monitoring, etc. Hierarchical nanocomposites and polymer-nanoreinforcement interactions.
- **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)
- X-Ray Characterization of Materials (Dr. F. Sket)
- 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 and TiAl based alloys for the next generation of turbine blades, FeAl alloys for steam turbines.

- **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.

- **Solidification and Casting:** optimization of casting processes and solidification-microstructure relationships using traditional (vacuum induction melting, vacuum arc melting, gravity and tilt casting, directional solidification) and advanced techniques (centrifugal and suction casting, vacuum melt atomization)

- **High strength steels:** development of novel thermo-mechanical processing routes for fabrication of quenched and partitioned steels with superior mechanical properties, analysis of processing-microstructure-properties relationship on macro- and micro-scales with emphasis on their strength, ductility, and fatigue and fracture resistance.

- **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 (rolling, forging, extrusion, welding, casting, etc.).

- **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 macro mechanical properties.

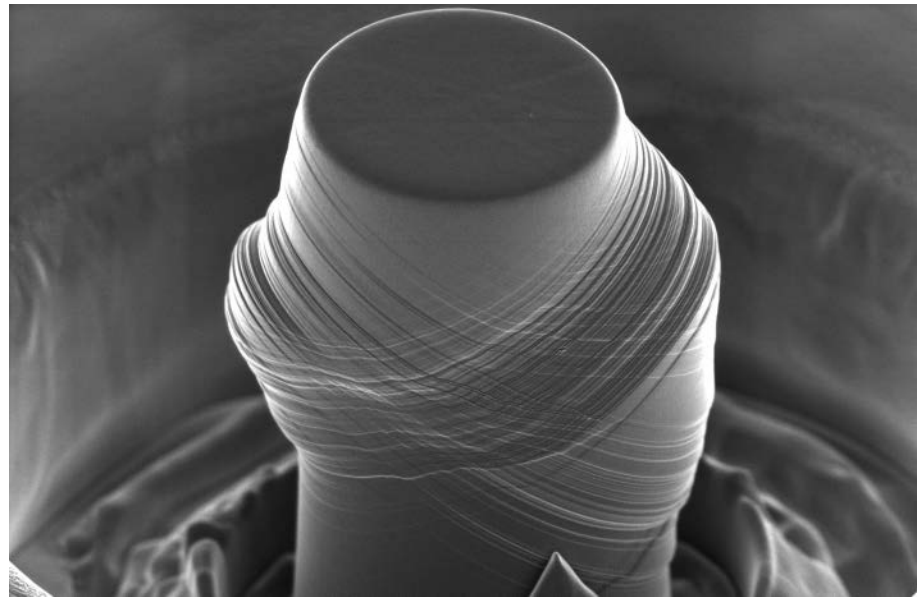
- **Model-based materials design:** integrating Molecular Dynamics, computational thermodynamics and kinetics, and mesoscale modeling (Landau/Phase Field) of microstructure for materials & processing design.

- **Simulation of the mechanical behaviour:** 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.

- **Solid state processing:** development of new alloys by thermo-dynamical approaches and by powder manufacturing via mechanical alloying and gas atomizing in non-oxidation conditions. Consolidation by field-assisted sintering and conventional press and sintering.

Research groups involved:

- Physical Metallurgy (Dr. M. T. Pérez-Prado, Programme Leader)
- Solid State Processing (Prof. J. M. Torralba)
- Solidification Processing and Engineering (Dr. S. Milenkovic)
- Physical Simulation (Dr. I. Sabirov)
- Multiscale Materials Modeling (Dr. J. Segurado)
- Computational Alloy Design (Dr. Y. Cui)
- X-Ray Characterization of Materials (Dr. F. Sket)
- High-Temperature Alloys (Dr. Carl Boehlert)



Integrated Computational Materials Engineering

ABENGOA RESEARCH

- **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.),
  - Metals under extreme conditions (Fe, FeCr, FeC, W)
  - Materials for energy generation and storage.

- **Materials modelling at different length and time scales:**
  - First principle calculations
  - Molecular mechanics and molecular dynamics
  - Dislocation dynamics
  - Object and lattice Kinetic Monte Carlo
  - Computational thermodynamics and kinetics
  - Microscale-mesoscale-structural scale modelling (Landau/Phase field)
  - Numerical methods for solids (finite elements and other approximations for solid mechanics)
  - Computational micromechanics, computational mechanics
  - Modelling and simulation of multiscale transport phenomena (application to advanced materials for batteries)

- **Multiscale materials modelling:**
  - Bottom-up approaches (scale bridging)
  - Development of modular multi-scale tools
  - High throughput screening integration
  - Concurrent models
  - Homogenization theory

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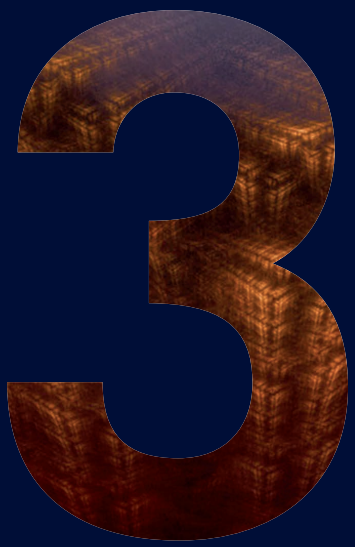
AIRBUS DEFENCE & SPACE

Fokker

Research groups involved:

- Atomistic Modelling of Materials (Dr. I. Martin-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



annual report 2014

The IMDEA Materials Institute is committed to attracting talented researchers from all over the world to Madrid to work in an international and multidisciplinary environment. The Institute currently has 16 staff researchers, three visiting researchers, 21 post-doctoral researchers and 40 doctoral students from 16 different nationalities, plus 20 post-graduate students studying for a master's degree. It should be noted that 42% of the researchers are foreign nationals, while 57% of the PhDs awarded were granted by foreign universities. Such an international team, and with such multidisciplinary expertise, is contributing to establishing the Institute as an international reference in materials science and engineering. The researchers are supported by six laboratory technicians and management and administrative staff, including an International Project Office.

Its research team makes the Institute a unique centre in Spain for two main reasons. The first one is the real international environment in which researchers from 16 different nationalities work together. And the second is the breadth of its coverage of materials science and engineering by the extent of its multidisciplinary approach. In fact, formal qualifications of the research staff come from the academic fields of chemistry, engineering (aeronautical, civil, mechanical and electrical), materials science, metallurgy and physics.

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 carry out virtual design, virtual processing and virtual testing of engineering materials for structural applications; 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. 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.

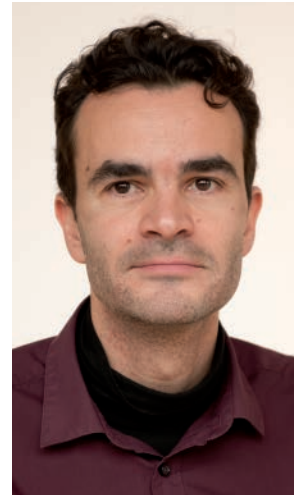
Dr. Ignacio Martin-Bragado

Senior 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. 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. Yuwen Cui

Senior 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.

Prof. Ignacio Romero

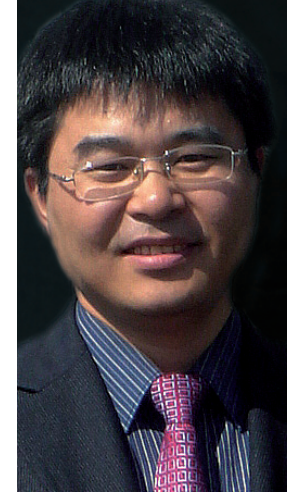
Senior Researcher, Computational Solid Mechanics

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

Professor of Mechanical Engineering, Technical University of Madrid

Research Interests

Numerical methods for nonlinear mechanics of solids, fluids, and structures. Development of time integration methods for Hamiltonian and coupled problems, models and numerical methods for nonlinear beams and shells, improved finite elements for solid mechanics, error estimators in nonlinear dynamics and multiscale methods for material modeling.



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. 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. 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 nanostructure materials, design and processing of high performance polymers and their nanocomposites, with particular emphasis in structural properties and behaviour under fire.

researchers

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. Federico Sket

Researcher, X-ray characterization of materials

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. 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

Dr. Yun Liu

Visiting Scientist, Bio-based fire retardant materials

Ph.D. in Polymeric Chemistry from Sichuan University. China

Associate Professor. College of Chemistry and Chemical Engineering. Wuhan Textile University. China

Research Interests

Halogen-free flame retardant textile and polymeric materials, flame retardant nano-materials, preparation and characterization of biocompatible and biodegradable polymer composites.

Prof. Qinghong Kong

Visiting Scientist, Eco-friendly Fire Retardant Materials

Associate Professor, School of environmental and safety engineering, Jiangsu University

Research Interests

Synthesis, characteristation and properties of inorganic nanomaterials. Preparation of polymer/inorganic nanocomosites, and analysis their structure and properties. Thermal and combustion performance of flame retardant polymer nanocomposites.

Prof. Jiang Wang

Visiting Scientist, Experimental determination of phase equilibria

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

Professor. Guilin University of Electronic Technology (GUET), School of Materials Science and Engineering. China

Research Interests

Experimental determination of phase equilibria, kinetics and magnetic properties, thermodynamic calculation and diffusion kinetic simulation, microstructure evolution of alloys using integrated computational materials method.

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. 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. Juan Pablo Balbuena

Postdoctoral Research Associate

Ph.D. in Physics from Physics from Autonomous University of Barcelona. Spain

Research Interests

Kinetic Monte Carlo (KMC) simulation of diffusion and activation/deactivation of dopants, impurities and radiation-induced defects in silicon, and germanium-based materials used in microelectronics, lattice KMC modelling of epitaxial processes in Si, Ge and III-V semiconductors, ensemble Monte Carlo simulation of bulk properties in semiconductors, drift-Diffusion approximation model for charge carriers transport in semiconductor devices, hybrid CPU-GPU parallel C++ programming algorithms.

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. 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 modeling (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. Carmine Coluccini
Postdoctoral Research Associate

Ph.D. in Chemical Science from Università di Bologna. Italy.

Research Interests
Organic synthesis, design and synthesis of organic and organometallic dyes for DSSC, and organometallic complexes as electrolytes for DSSC; aromatic fluorescent polymers, supramolecular chemistry.

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), modeling of fretting and wear, structural integrity.

Dr. Olben Falcó
Postdoctoral Research Associate

Ph.D. in Mechanical Engineering from University of Girona. Spain

Research Interests
Design of advanced composites laminates with non-conventional architectures manufactured by means of advanced fiber placement. Numerical analysis and simulation of progressive damage and failure in variable stiffness composite panels. Experimental studies of "Tow-drop" defects under in-plane and impact loading. Damage resistance and damage tolerance analysis in variable stiffness composite panels.

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. David González
Postdoctoral Research Associate

Ph.D. in Materials Science and Engineering from the University of Manchester. UK

Research Interests
Crystal plasticity, modelling of damage, deformation and stress.

Dr. Vignesh Babu Heeralal
Postdoctoral Research Associate

Ph.D. in Chemistry from University of Hyderabad. India

Research Interests

High performance flame retardant polymer composite and/or nanocomposites, polymer composites processing and manufacture, environmentally friendly thermoset polymers from renewable feedbacks.

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. Dong-Wook Lee
Postdoctoral Research Associate

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

Research Interests

Phase field modeling of solid-state phase transformation, mesoscale modeling of 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. Andrey Sarikov
Postdoctoral Research Associate

Ph.D. in Solid State Physics from V. Lashkarev Institute of Semiconductor Physics. NAS Ukraine. Ukraine

Research Interests

Thermodynamics and kinetics of phase separation in the non-stoichiometric silicon oxide films, thermodynamics and kinetics of the metal induced crystallisation of amorphous and disordered Si, Monte Carlo modelling of the formation and transformation of semiconductor structures.

Dr. Diego Fernando Mora
Postdoctoral Research Associate

Ph.D. in Structural analysis from Polytechnic 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. Bin Tang
Postdoctoral Research Associate

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

Research Interests

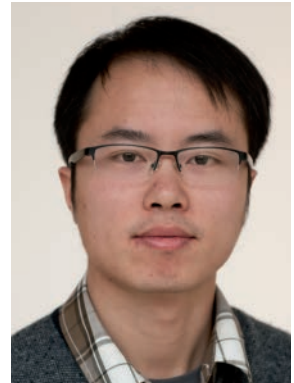
Phase field modeling of phase transformation in metals, solid phase transformation and relationship between microstructure evolution and mechanical properties in high strength Ti alloys, thermal deformation and solid-state diffusion bonding of γ-TiAl alloys, finite element simulation of plastic deformation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

Dr. 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.

Dr. Jian Xu

Postdoctoral Research Associate

Ph.D. in Computational Science in Enginering from University of Leuven. Belgium

Research Interests

Quasi-static and fatigue damage modelling/experiment, multiscale modelling impact modelling, impact and Damage Tolerance analysis of composite structures

Dr. Jun-Hao Zhang

Postdoctoral Research Associate

Ph.D. in Inorganic Chemistry from University of Science and Technology of China. China

Research Interests

Design, synthesis and properties of functional inorganic materials, mass preparation of inorganic materials, high performance, flame retardant polymer-based nanocomposites.

research assistants

Laura Agudo

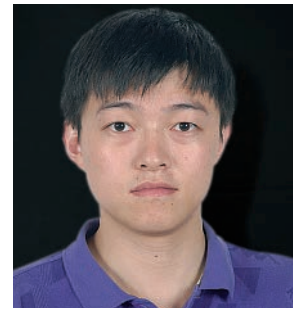
MEng: Rey Juan Carlos University. Spain
Research: Multiscale materials modelling

Marta Cartón

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

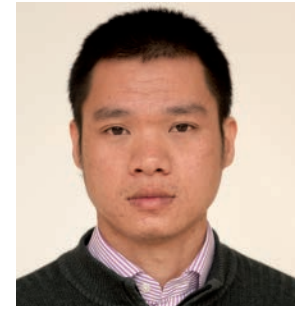
Almudena Casado

MSc: Carlos III University of Madrid. Spain
Research: Solidification and casting



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

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

Momchil Jeliazkov

MEng: Delft University of Technology. The Netherlands
Research: Buckling and Failure Optimization of Stiffened Tow-steered composite panels

Sergio de Juan

BEng: Technical University of Madrid, Spain
Research: High performance nanocomposites

Daniel del Pozo

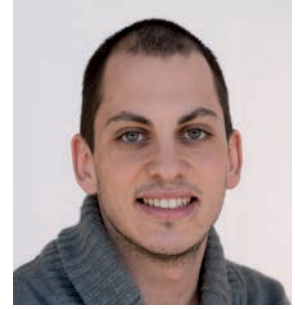
BEng: Technical University of Madrid, Spain
Research: Modeling of ice impact on jet turbines

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



Juan Carlos Fernández

MSc: Carlos III University of Madrid. Spain
Research: Electric curing of carbon nanotubes/epoxy resins

Alejandro García

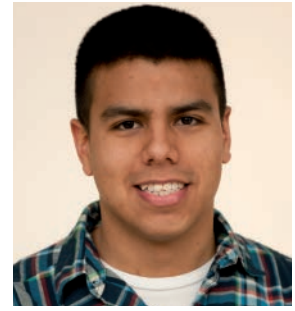
MEng: Carlos III University of Madrid. Spain
Research: High energy impact on aeronautical composite structures

José Luis Gómez-Sellés

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

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

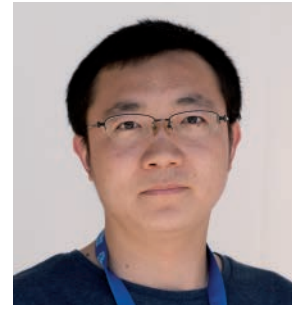
MEng: Isfahan University of Technology. Iran
Research: Solid state processing of metallic alloys

Marcos Jiménez

MEng: Carlos III University of Madrid. Spain
Research: Micromechanics of Ni superalloys

Ehsan Naderi Kalali

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



Zhi Li

MSc: Shanghai Jiang Tong University. China
Research: New generation fire retardant materials

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

Mohammad Marvi-Mashhadi

MSc: Ferdowsi University of Mashhad. Iran
Research: Multiscale modelling of polyurethane foams

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

Peyman Mouri

MEng: Delft University of Technology. The Netherlands
Research: Characterization, design and optimization of dispersed-ply laminates

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

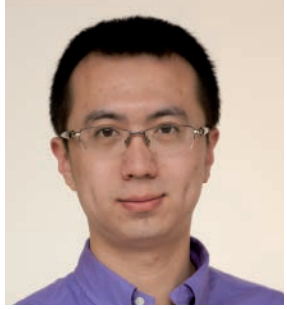
MEng: Carlos III University of Madrid. Spain
Research: Computational mechanics of composite materials

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

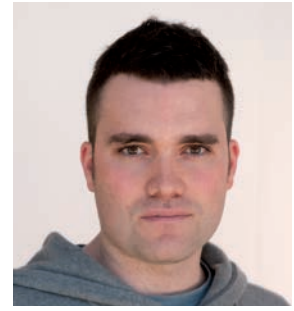
MEng: Technical University of Madrid. Spain
Research: Multiscale plasticity

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

Evgeny Senokos

MEng: Lomonosov Moscow University. Russia
Research: Nanostructured supercapacitors

Rafael Soler

MSc: Cranfield University. UK
Research: Nanomechanics

Juan José Torres

MEng: Tecnun. Spain
Research: Voids in out-of-autoclave prepregs

Arcadio Varona

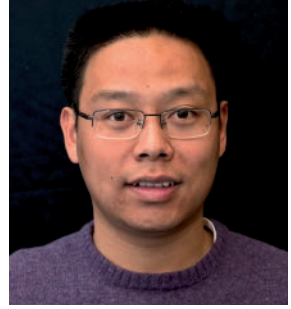
MEng: Rey Juan Carlos University. Spain
Research: Advanced NiAl-based eutectic alloys

Joaquim Vilà

MEng: University of Girona. Spain
Research: Processing of composites by infiltration

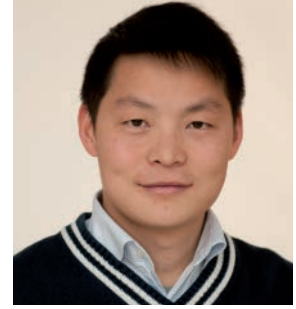
Chuanyun Wang

MSc: Northwestern Polytechnical University. China
Research: High throughput diffusion and phase transformation



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

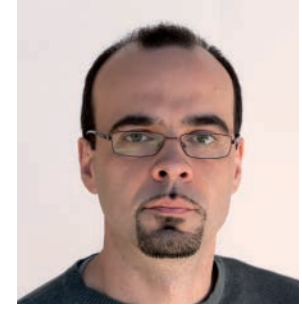
laboratory technicians

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

David Maldonado

MEng: University of Valencia. Spain

general management

Dr. Covadonga Rosado
Manager

Rosa Bazán
Personnel Manager

Eduardo Ciudad-Real
Accountant Responsible

Vanessa Hernán-Gómez
Accountant Assistant

Elena Bueno
Executive Secretary

Mariana Huerta
Administrative Assistant

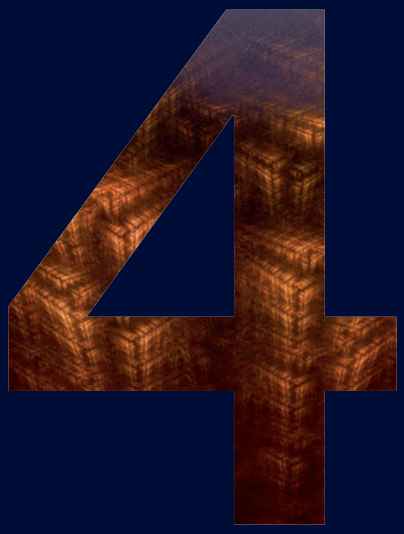
international project office

Miguel Ángel Rodiel
Technology Manager &
Project Office Responsible

Dr. Germán Infante
R&D Project Manager

Borja Casilda
Administrative Assistant

research infrastructure



annual report 2014

4.1. New research infrastructure

The following facilities became operational along year 2014. They are further described in the following sections):

- **Dual column universal testing system** (INSTRON 5966)
- **Fatigue testing system** (INSTRON 8802)
- **Drop weight impact test system** (INSTRON CEAST 9350)
- **Fiber mechanical testing machine** (FAVIMAT+, Textechno)
- **Planetary mills** (FRITSCH PULVERISETTE 6 classic & 7 premium)
- **Micro-scale combustion calorimeter** (Fire Testing Technology)
- **In situ Nanoindenter Stage** (PI87, Hysitron)

4.2. Processing

- **Planetary Mills (2014 new equipment)** (Fritsch Pulverisette 6 classic & 7 premium) for the finest rapid, batchwise comminution of hard to soft grinding material, dry or in suspension, down to colloidal or nanometer fineness. Maximum sample quantity: 225 ml (model 6 classic), 70 ml (model 7 premium). Rotational speed of main disk up to 1000 rpm (model 7 premium). Areas of application include mechanical alloying, metallurgy, ceramics, chemistry, etc.

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

- **Extruder** (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 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 (Tmax=1200 °C).

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

- **Three-Roll Mill** (Exakt 80 E, Exact Technologies) to disperse fillers and additives in viscous matrix. The shearing forces to break agglomerate are generated by three hardcrome-plated rollers that rotate at different angular velocities and where gap (minimum 5 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.

4.3. Microstructural Characterization

- **FIB-FEGSEM Dual-Beam Microscope** (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** (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.

4.4. Mechanical Characterization

- **Dual Column Universal Testing System (2014 new equipment)** (INSTRON 5966) to perform mechanical tests (including tension and compression, shear, flexure, peel, tear, cyclic and bending).The INSTRON 5966 model has 10 kN of capacity and 1756 mm of vertical test space.

- **Fatigue Testing System (2014 new equipment)** (INSTRON 8802). Servo-hydraulic mechanical testing machine (maximum load of 250 kN) with precision-aligned, high-stiffness load frames to carry out a broad range of static and dynamic tests from small coupons to large components. It is equipped with an environmental chamber for mechanical tests between -150ºC and 350ºC.

- **Drop Weight Impact Test System (2014 new equipment)** (INSTRON CEAST 9350) designed to deliver impact energies in the range 0.6 to 757 J. This instrument can be used to test any type of materials from composites to finished products, and is suitable for a range of impact applications including tensile impact.

- **Fiber Mechanical Testing Machine (2014 new equipment)** (FAVIMAT+, Textechno) to characterize fiber mechanical properties, as well as linear density and crimp. Measurement of the mechanical properties in a liquid medium is also possible.

- **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.

- **In situ Nanoindentation Stage** (PI87, Hysitron) to carry out mechanical tests inside a scanning electron microscope (SEM) for the *in situ* observation of the deformation mechanisms. The stage allows the simultaneous acquisition of the load-displacement record and the SEM images during mechanical testing (nanoindentation, micro-compression, micro-bending, micro-tension) of micrometer and sub-micrometer size volumes, including elevated temperature testing.

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

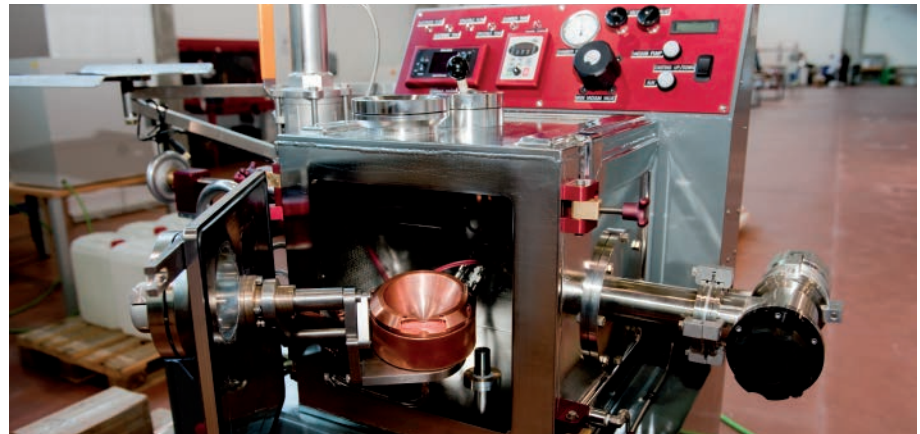
- **Rheometer** (AR2000EX, TA Instruments) to determine the rheological behaviour and viscoelastic properties of fluids, polymer melts, solids and reactive materials (resins) in the temperature range 25ºC to 400ºC.

4.5. Thermal Characterization

- **Micro-scale Combustion Calorimeter (2014 new equipment)** (Fire Testing Technology) to carry out laboratory scale tests of the flammability of materials with milligram quantities. The tests provide the peak heat release rate, the total heat released, the time to the peak heat release rate and the heat release capacity of the material. The samples are tested according to ASTM standard D7309-07.

- **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.

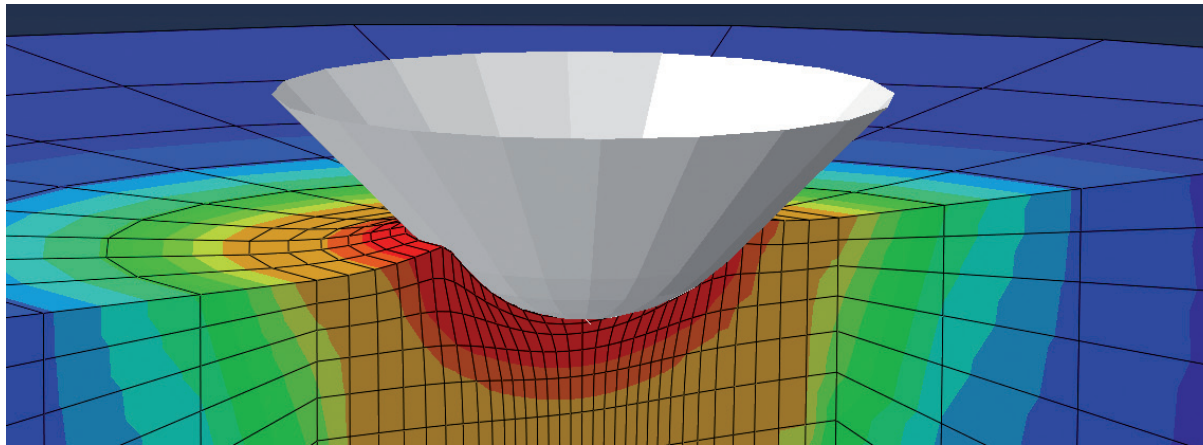
- **Differential Scanning Calorimeter** (Q200, TA Instruments) to analyse thermal properties/phase transitions of different materials up to 725ºC. Equipped with Tzero technology, it provides highly reproducible baselines, superior sensitivity and resolution. It is also coupled with a cooling system to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

- **Thermogravimetric Analyzer** (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 Furnaces** (Nabertherm, RHTH 120/600/16) to carry out heat treatmentsup to 1600ºC in vacuum or inert atmosphere and 2 Carbolite, CWF 1300 for heat treatments in air up to 1300ºC.

4.6. Simulation

- High performance computing cluster 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.).



In-house developed codes

MMonCa ©

Open Source Kinetic Monte Carlo simulator developed by the Atomistic Modelling of Materials group and collaborators. It contains a Lattice KMC module, used mainly for simulation of epitaxy, and an off-lattice Object KMC module for simulation of damage irradiation in simple elements (Si, Ge, Fe, Cu...), binary compounds (SiC, GaAs) and alloys (FeCr, SiGe). The Kinetic Monte Carlo simulator is coupled to a finite element code to include the effect of mechanical stresses, and to an Ion Implant Simulator. Download at http://www.materials.imdea.org/MMonCa

CAPSUL ©

CAPSUL is a package of crystal plasticity and polycrystalline homogenization simulation tools. The package includes:

A crystal plasticity model, aimed to predict the elasto-plastic behaviour at the crystal level, taking into account the actual deformation mechanisms for a particular metal (slip, twinning...). The model incorporates several flow rules and accounts for isotropic hardening, kinematic hardening, cyclic softening and ratchening. These features allow the study of monotonic and cyclic loading. The model has already been successfully used in FCC alloys (Al, Ni-based superalloys), and HCP (Mg and Ti) alloys to predict quasistatic behaviour, texture evolution and fatigue performance.

A tool to generate representative volume elements taking into account the microstructural features (grain size, shape and orientation distribution).

An inverse optimization tool to obtain the parameters that dictate the single crystal behavior from the result of macroscopic mechanical tests in polycrystals.

VIPPER ©

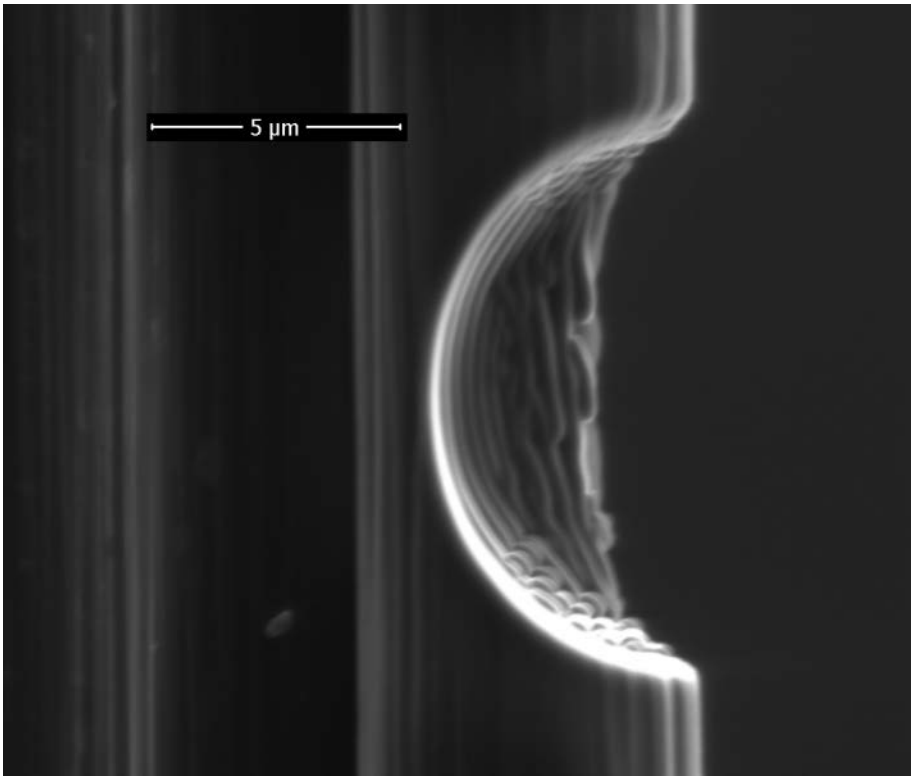
A simulation tool developed within the framework of computational micromechanics by IMDEA Materials Institute to predict ply properties of fiber-reinforced composite materials from the properties and spatial distribution of the different phases and interfaces in the composite. The tool is also able to generate composite microstructures with arbitrary

fibre geometries as well as hybrid microstructures hence allowing for in-silico ply property design and optimization.

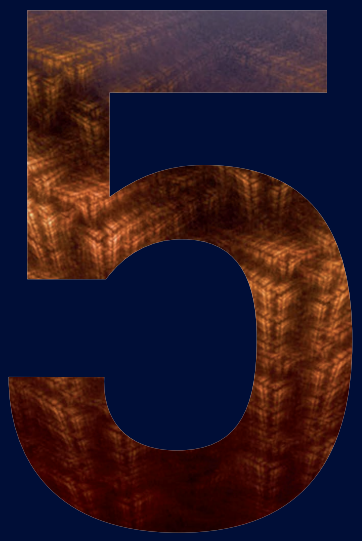
Moreover, IMDEA Materials Institute has developed other in-house codes for modelling and simulation of thermodynamic properties and phase-diagrams as well as mechanical behaviour and damage evolution of engineering materials.

4.7. 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

2014

The year 2014 has been an excellent one for the IMDEA Materials Institute both in terms of the number of projects awarded and funding. The institute has participated in 55 research projects, 19 of which began during the year. With respect to project funding, 2014 experienced a year-on-year increase of 32%. In particular, project funding coming from European projects and industrial contracts increased by 33% and 12% respectively. It should also be highlighted that funding from national calls increased by 173% year-on-year.

The project portfolio is divided into three main groups: 26 projects were obtained in international competitive calls, out of which 16 were funded by the EU, seven by the China 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. Nine projects are supported by research programmes sponsored by MINECO and two by the Regional Government of Madrid, while 18 projects are directly funded through industrial contracts. Several of these industrial contracts are supported by the Spanish Centre for the Development of Industrial Technology (CDTI).

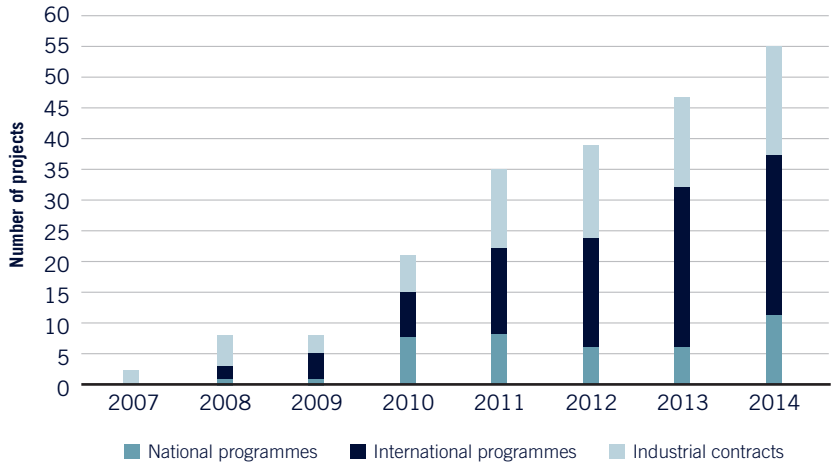
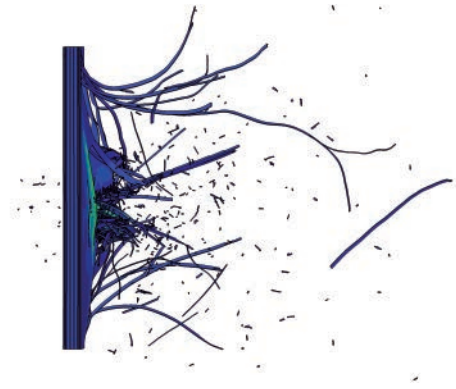


Figure 4. Number of active research projects during 2014 by funding source

A brief description of the projects started in 2014 is provided below:

CRASHING

"Characterization of structural behaviour for high frequency phenomena"



Funding: **Clean Sky Joint Undertaking, European Union-7th Framework Programme**
Partners: IMDEA Materials Institute (Coordinator) and Carlos III University of Madrid
Duration: **2014-2016**
Principal Investigator: **Dr. C. S. Lopes**

The use of composite materials as principal structural elements in an aircraft requires the complete understanding of their mechanical properties particularly under impact. The main objective of the CRASHING project is to develop a multiscale model approach that takes into account the physical mechanisms of damage at the different length scales. The multiscale approach describes systematically the material behaviour at ply, laminate and component levels. Final models of the multi-scale approach will be suitable for simulations of aircraft crash-landing, ditching, bird strike, ice impacts and, in general, situations where the aircraft is subject to high frequency dynamic loading.

This ambitious two-year research project, funded by the Clean Sky Joint Technology Initiative (JTI-Clean Sky) within the 7th Framework Programme of the European Union, is led and coordinated by the IMDEA Materials Institute which is responsible for the development and validation of the multiscale models at the micro, meso and structural levels. The other partner of the consortium, Carlos III University of Madrid is in charge of the experimental characterisation of materials under impact.

DESMAN

"New structural materials for energy harvesting and storage"

Funding: **B/E Aerospace Inc (USA)**
Partners: IMDEA Materials Institute (coordinator) and IMDEA Energy Institute
Duration: **2014-2017**
Principal Investigator: **Dr. J. J. Vilatela**

DESMAN is a three-year industrial contract with the US company B/E Aerospace Inc., the worldwide leading manufacturer of aircraft passenger cabin interior products, to develop

innovative materials for aircraft interiors based on advanced polymers and macroscopic fibres. The aim is to exploit the multifunctional properties of these fibres and their unique hierarchical structure to produce lighter aircraft structures with multifunctional capabilities. The project is led by the Multifunctional Nanocomposites group at IMDEA Materials Institute and developed jointly with IMDEA Energy Institute.

AROOA

"Study of the factors influencing air removal in out-of-autoclave processing of composites"

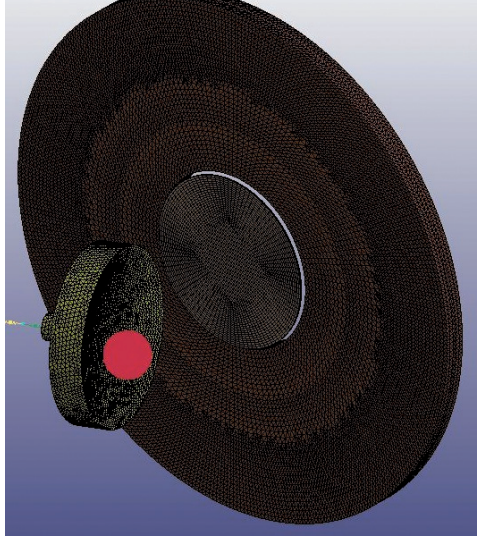
Funding: **Hexcel Composites Limited (UK)**
Duration: **2014-2017**
Principal Investigators: **Dr. C. González and Dr. F. Sket**

AROOA project aims to study and optimize a new family of prepregs designed for out-of-autoclave processing of composite materials in collaboration with Hexcel. This new technology allows savings in the manufacturing of components and structures for aircrafts. AROOA project will be carried out by the Structural Composites and Nanomechanics groups of IMDEA Materials Institute, integrating their know-how in advanced characterization and modelling.

SIMUFOING

"Development and validation of simulation methods for ice and bird ingestion in airplane engines"

Funding: **Industria de Turbo Propulsores S.A. (ITP)**
Duration: **2014-2015**
Principal Investigator: **Dr. I. Romero**



The project SIMUFOING between IMDEA Materials and Industria de Turbopropulsores (ITP) is aimed at the development of new simulation techniques that can be used to predict damage on aircraft engines due to the ingestion of hailstones and birds. The numerical methods will be validated with experimental data provided by ITP, and should be accurate enough to estimate structural failure of engine parts at a wide range of ingestion velocities. The Computational Solid Mechanics group at IMDEA Materials will be responsible for the dynamic simulations and the material model implementation.

GRUPO FerroAtlántica

SICASOL

"Solar-grade silicon: purification in high vacuum furnace"

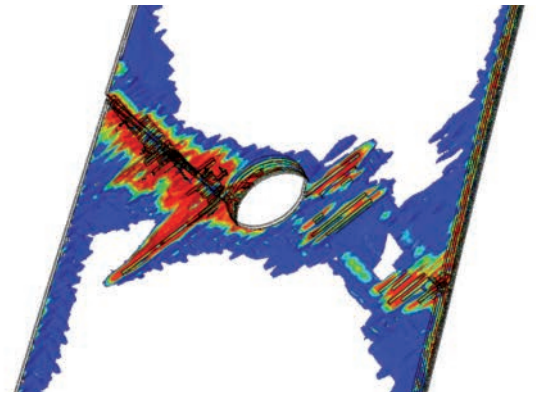
Funding: **Silicio Ferrosolar S.L (FerroAtlántica Group) and Spanish Centre for Industrial Technological Development (CDTI)**
Duration: **2014-2015**
Principal Investigators: **Prof. J. M. Torralba and Dr. Milenkovic**

The demand of raw materials for the photovoltaic industry is growing fast. Solar-Grade Si (SGS) is the main material for the manufacturing of solar cells. The most convenient method of obtaining SGS is the purification of metallurgical-grade Si but this route is hindered by several problems (condensation of contaminated Si in the furnace walls and degradation of refractory material due to thermal shock or chemical degradation) that arise during the production of SGS via impurities evaporation (mainly B and P) in a high vacuum furnace. SICASOL project aims at optimizing the production process of SGS by minimizing the impact of these problems in the production process.

VIRTEST

"Multiscale virtual testing of CFRP samples"

Funding: **Fokker Aerostructures B.V.**
Duration: **2014-2016**
Principal Investigator: **Dr. C. S. Lopes**

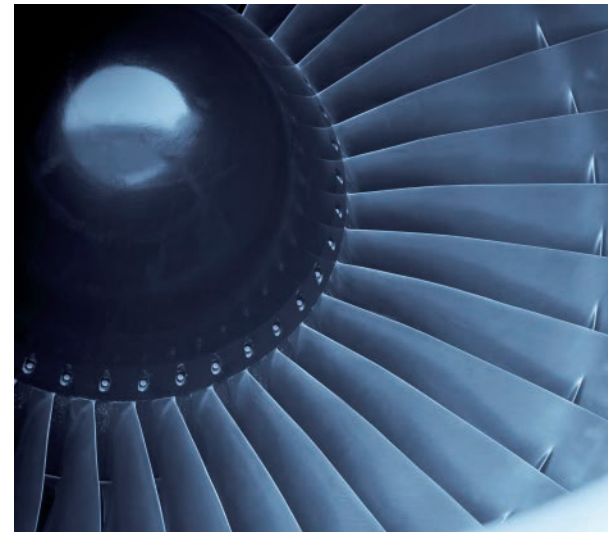


IMDEA Materials and Fokker Aerostructures collaborate under the bilateral project VIRTEST to develop a novel multiscale simulation strategy to predict the mechanical behaviour of aeronautical composite laminates structures under static and low-velocity impact loads. VIRTEST will lead to a significant reduction in the number of physical tests required for material certification and will shorten the time necessary to design new aerospace structural components at Fokker.

XMART

"Study of the effect of porosity and its distribution on MAR-M-247 tensile and fatigue test specimens"

Funding: **Industria de Turbo Propulsores S.A. (ITP)**
Duration: **2014-2015**
Principal Investigators: **Dr. F. Sket and Dr. J. Molina**

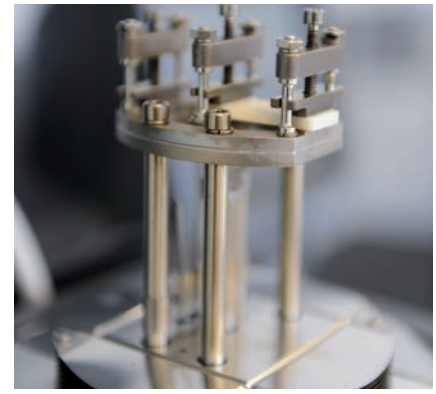


The XMART project is an industrial collaboration with Industria de Turbopropulsores S. A aiming at studying the effect of porosity and its distribution on the mechanical behaviour under static and cyclic loads of MAR-M-247 specimens. The porosity will be characterized by means of X-ray computed tomography for further correlation with the fracture surface and the mechanical tests. XMART project will be carried out by the research group on X-ray characterization of Materials of IMDEA Materials Institute taking advantage of the know-how in advance characterization of materials and image analysis techniques.

DMAPOL

"Dynamic mechanical analyses in polymeric materials"

Funding: **ACCIONA Infraestructuras S.A.**
Duration: **2014**
Principal Investigator: **Dr. J. P. Fernández**

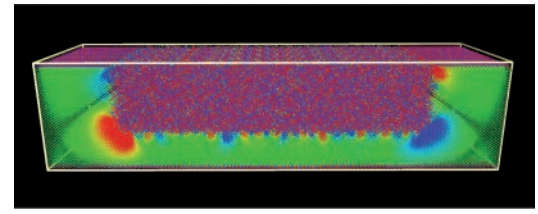


DMAPOL is an R&D collaboration between ACCIONA Infraestructuras and IMDEA Materials Institute to characterize the viscoelastic properties of composite laminates used in building industry. The goal is to study the thermal behaviour of the thermostable resins once the laminate has been conformed.

EPISIM

"Simulation of epitaxial growth"

Area: **Asia / Pacific**
Duration: **2014-2016**
Principal Investigator:
Dr. I. Martin-Bragado



The goal of this project, led by the Atomistic Modeling of Materials group, is to develop Lattice Kinetic Monte Carlo models for our Open Source MMonCa simulator to analyze atomistic mechanisms in semiconductor materials for the next generation of microelectronic devices.

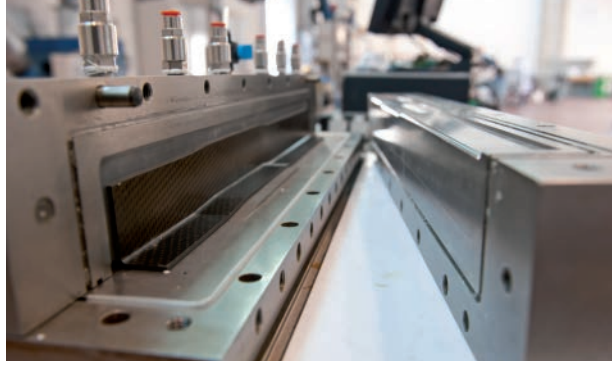
ONLINE-RTM

"Online NDT RTM inspection in composites"

Funding: **Airbus Operations S.L.**
Duration: **2014-2015**
Principal Investigator: **Dr. C. Gonzalez**

ONLINE-RTM is a research collaboration between IMDEA Materials and Airbus Operations aiming at analysing sensor information during RTM injection to asses quality of com-

posite parts. The incorporation of this new technology in the manufacturing process will lead to a reduction of cost because the need for an exhaustive non-destructive inspection after manufacturing will be reduced.

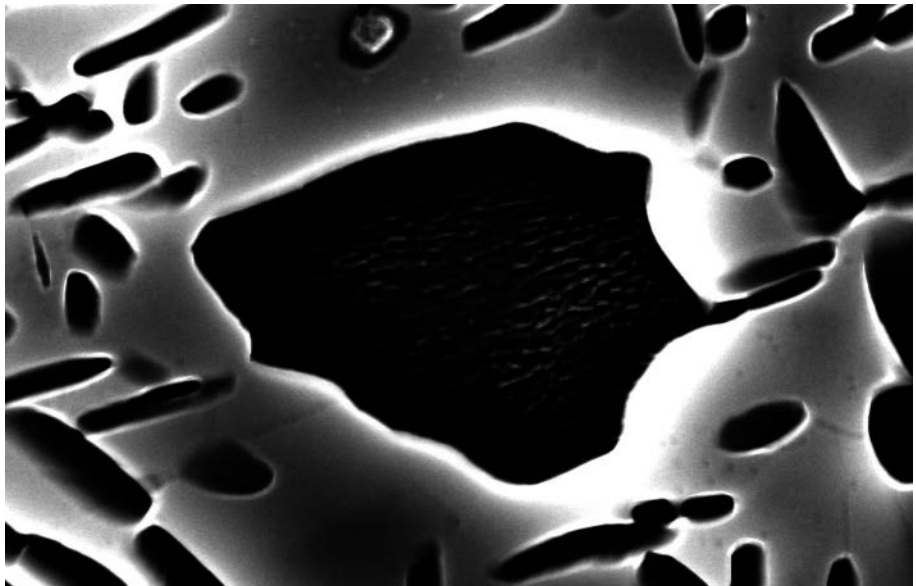


DIMMAT

"Multiscale design of advanced materials"

Funding: **Regional Government of Madrid**
Partners: IMDEA Materials Institute (Coordinator), National Centre for Metals Research (CSIC), Institute for Materials Science (CSIC), Institute for Nuclear Fusion of the Technical University of Madrid, Department of Materials Science, Technical University of Madrid, Carlos III University of Madrid and Complutense University of Madrid.
Duration: **2014-2018**
Principal Investigator: **Dr. M. T. Perez-Prado**

The main aim of DIMMAT is to leverage the complementary capabilities of several research groups of the Madrid region in order to configure a novel methodology for materials design that is more efficient than traditional ones based in trial and error methods. To achieve this ambitious goal, the DIMMAT consortium, coordinated by IMDEA Materials Institute, provides a multidisciplinary perspective which brings together expertise of seven research groups in Madrid in computational materials design, materials modelling, processing and characterization. The activities are carried out in collaboration with several companies, leaders in their respective sectors, such as Airbus, the Antolín Group, Industria de Turbopropulsores, Abengoa, Sandvik and Acerinox. The methodology for materials innovation that will be developed in the frame of the project will be applied to optimize the properties of several metallic materials and polymer-based composites, with applications in construction, transport and energy industries.



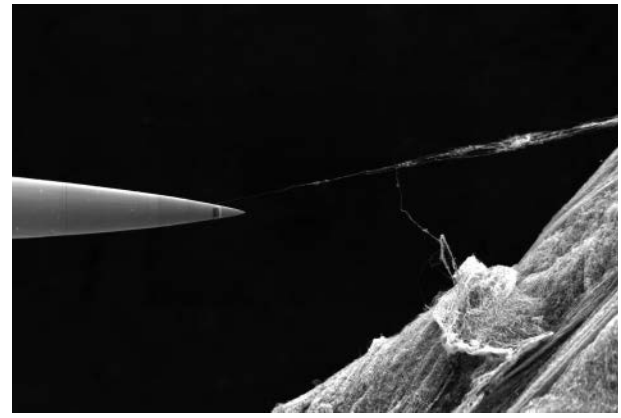
La Suma de Todos
Comunidad de Madrid
www.madrid.org

EUROPEAN UNION
STRUCTURAL FUNDS

MAD2D

"Fundamental properties and applications of graphene and other bidimensional materials"

Funding: **Regional Government of Madrid**
Partners: Institute of Materials Science of Madrid (CSIC) (Coordinator), IMDEA Nanoscience Institute, IMDEA Materials Institute, IMDEA Energy and Autonomous University of Madrid.
Duration: **2014-2018**
Principal Investigators: **Dr. J. J. Vilatela and Dr. J. Molina**



The main goal of MAD2D programme is to study the properties of graphene, other bidimensional materials and related structures, with emphasis on the development of devices for energy management and sensing. The project will be carried out by a team of five institutions in Madrid, with expertise ranging from fundamental physics of nanomaterials to the fabrication of macroscopic devices made up of nanostructured building blocks.

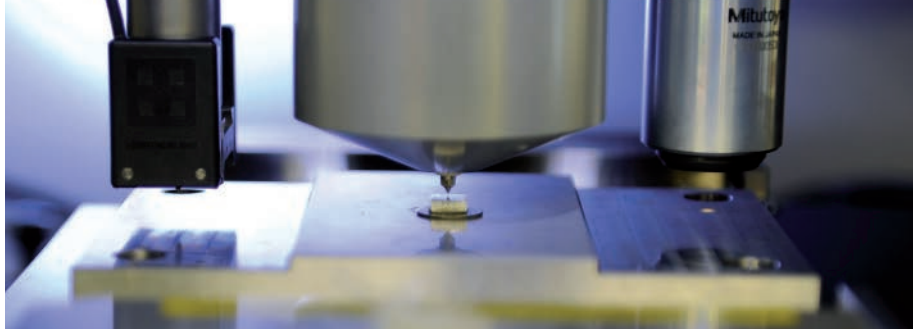
The principal role of IMDEA Materials Institute in MAD2D is in the synthesis of nanocarbon/semiconductor hybrids for energy and sensing applications. These include photocatatalysts for CO_2 valorisation and hydrogen production, all-solid pseudocapacitors, and mesoporous nanostructured sensors.

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Ferro-GENESYS

"Heat resistant Fe-base alloys for application in generation energy systems"

Funding: **Spanish Ministry of Economy and Competitiveness**
Partners: National Centre for Metals Research (CSIC) (Coordinator), Centre for Energy Research (CIEMAT), IMDEA Materials Institute, Centre of Technical Studies and Research and Carlos III University of Madrid.
Duration: **2014-2017**
Principal Investigator: **Dr. I. Martin-Bragado**



Within the framework of the coordinated project Ferro-GENESYS, IMDEA Materials Institute will model irradiation damage and carry out the nanoscale mechanical characterisation of ODS FeCrAl and FeAl(Cr/Zr) heat resistant alloys. The following specific objectives will be considered: i) development of modelling codes aimed at predict the radiation damage effect on the FeCr microstructure. The MMonCa simulator developed at IMDEA Materials will be extended to include at the same time models for the interdiffusion of FeCr and the evolution of defects with time and temperature, ii) determination of mechanical properties by nanoindentation in nano/micro- structured FM steels, and ODS alloys, and iii) the characterization of ODS alloys by means of indentation creep (T < 850 ºC).

SEPIFIRE

"Study of sepiolite-based fire retardant systems"

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Funding: **Spanish Ministry of Economy and Competitiveness**
Partners: TOLSA S.A. and Institute of Materials Science of Madrid (CSIC)
Duration: **2014-2017**
Principal Investigator: **Dr. D.-Y. Wang**

In the SEPIFIRE project, the effect of functionalized sepiolite-based additives on fire retardancy of commercial polymer systems will be determined by different tests (Limiting oxygen index, vertical burning test, cone calorimeter, etc). The investigation will also include study of fire behaviour, fire retardant mechanisms, mechanical properties, thermal stability and structure of the char after burning.

GOBIERNO DE ESPAÑA MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

GAS

"Glasses and stability Excellence Network"

Funding: **Spanish Ministry of Economy and Competitiveness**
Partners: Nanomaterials and Microdevices group from the Autonomous University of Barcelona (Coordinator), Characterization of Materials group from the Polytechnic University of Catalonia (UPC), Polymer and Soft Materials group from Joint Centre University of the Basque Country University and the Spanish National Research Council, Laboratory of Low temperatures from the Autonomous University of Madrid, Brillouin Spectroscopy Laboratory from the Institute of Materials Science of Madrid and IMDEA Materials Institute.
Duration: **2014-2016**
Principal Investigator: **Prof. J. LLorca**

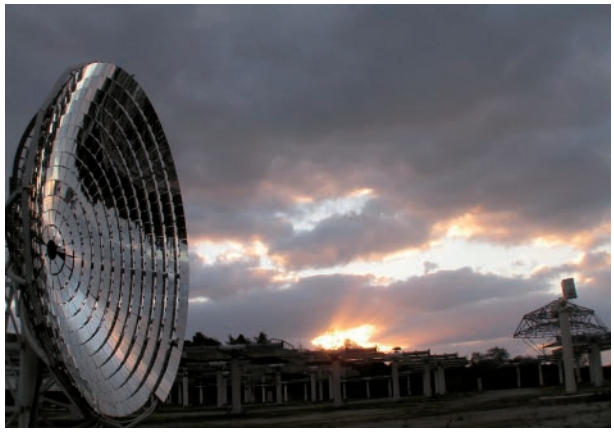
The collaborative effort of this network aims at increasing our basic understanding by studying glasses with very low-energy positions in the potential energy landscape. The success of the network will open de development of new applications on stable drugs, organic devices or metallic glasses with higher hardness and corrosion resistance.

GOBIERNO DE ESPAÑA MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

FOTOFUEL

"Solar fuels production challenges Excellence Network"

Funding: **Spanish Ministry of Economy and Competitiveness**
Partners: IMDEA Energy Institute (Coordinator), Institute of Catalysis and Petrochemistry, Institute of Chemical Research of Catalonia, IMDEA Materials Institute, ALBA, University of Barcelona, Jaume I University, Solar Platform of Almeria, MATGAS.
Duration: **2014-2016**
Principal Investigator: **Dr. J. J. Vilatela**



FOTOFUEL is a collaborative national network, coordinated by IMDEA Energy, which aims at promoting the development of materials and devices for the efficient production of solar fuels through the cooperation of several Spanish research groups with expertise in the fields of materials science, photocatalysis and simulation.

SCREENDM

"Screening of kinetic/microstructural information for Ti-alloys by diffusion multiple technique"

Funding: **China Scholarship Council**
Duration: **2014-2018**
Principal Investigator: **Dr. Y. Cui**

The project aims at developing a high-throughput diffusion technique for rapid screening of phase transformation kinetics and microstructure in Ti alloys. The idea is to generate a continuous multicomponent composition gradient by diffusion at high temperature (i.e. solid solutioning). The assembly is then subjected to a second thermal (i.e. ageing) and/or mechanical processes to create a morphology gradient arising from the compositional gradient. Kinetic information of phase transformations and microstructural development will be obtained from these tests for a wide range of compositions, so the most promising ones can be further analysed

CUCCOMP

"Development of Cu-C metal matrix composites"

Funding: **China Scholarship Council**
Duration: **2014-2015**
Principal Investigator: **Prof. J. M. Torralba**

The objective of this investigation is to develop copper-carbon composites which combine the properties of copper -high electrical conductivity and relatively good mechanical properties- with the low density of carbon, while the wear resistance is enhanced. Composites will be manufactured from copper and carbon powders (graphite and carbon nanotubes) consolidated by field-assisted sintering. The electrical conductivity, compressive strength and wear behaviour of the composites will be assessed.

OPE MADRIMASD

"European projects office madrimasd-IMDEA"

Funding: **Spanish Ministry of Economy and Competitiveness**
Duration: **2014-2017**
Project Responsible: **M. A. Rodiel**

The project aims at strengthening the European projects office Madrimasd IMDEA to support the participation of its members in European programs. The partners in this project are the institutes IMDEA Water, IMDEA Food, IMDEA Energy, IMDEA Materials, IMDEA Nanoscience , IMDEA Networks, IMDEA Software and Fundación para el Conocimiento madrimasd, which is the coordinator.

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

MATERPLAT

"Spanish technology platform of advanced materials and nanomaterials"

Funding: **Spanish Ministry of Economy and Competitiveness**
Duration: **2014-2015**
Project Responsible: **M. A. Rodiel**

IMDEA Materials is part of the coordination team of the Spanish technology platform of advanced materials and nanomaterials (MATERPLAT) with more than 160 associates from the private and academic sectors. MATERPLAT is a collaborative framework of exchange and communication among the different stakeholders of the Spanish system of science-technology-innovation. MATERPLAT aims at promoting innovation as a key tool to increase the competitiveness of the Spanish companies, for which advanced materials and nanomaterials are essential to keep or enhance their technological leadership.

Other ongoing research projects in 2014 at IMDEA Materials Institute were:

Clean Sky
SEVENTH FRAMEWORK PROGRAMME

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: **2013-2016**
Principal Researcher: **Dr. J. Segurado**

SEVENTH FRAMEWORK PROGRAMME

CARINHYPH "Bottom-up fabrication of nanocarbon-inorganic hybrid materials for photocatalytic Hydrogen production"

Funding: **NMP, European Union-7th Framework Programme**
Partners: IMDEA Materials Institute (Coordinator, Spain), Westfälische Wilhelms Universität Münster (Germany), Thomas Swan & Co Ltd. (United Kingdom), University of Cambridge (United Kingdom), Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany), INSTM (Italy), INAEL Electrical Systems (Spain) and EMPA (Switzerland)
Duration: **2013-2015**
Principal Investigator: **Dr. J. J. Vilatela**

PilotManu "Pilot manufacturing line for production of highly innovative materials"

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

SEMICURED STRINGERS "Highly integrated semi-cured parts"

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

COMPOSE3 "Compound semiconductors for 3D integration"

Funding: **ICT, European Union-7th Framework Programme**
Partners: IBM Research GmbH (Coordinator, Switzerland), STMicroelectronics-Crolles (France), Commissariat a l'Energie Atomique - Leti (France), University of Glasgow (United Kingdom), Tyndall National Institute (Irelan), Centre National de la Recherche Scientifique (France), DTF Technology GmbH (Germany) and IMDEA Materials Institute (Spain)
Duration: **2013-2016**
Principal Investigator: **Dr. I. Martín-Bragado**

ECURE "Electrically-curable resin for bonding/repair

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

NONCIRC "Non-circular carbon fibres"

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

ICMEG "Integrative computational materials engineering expert group"

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

NFRP "Nano-engineered fiber-reinforced polymers"

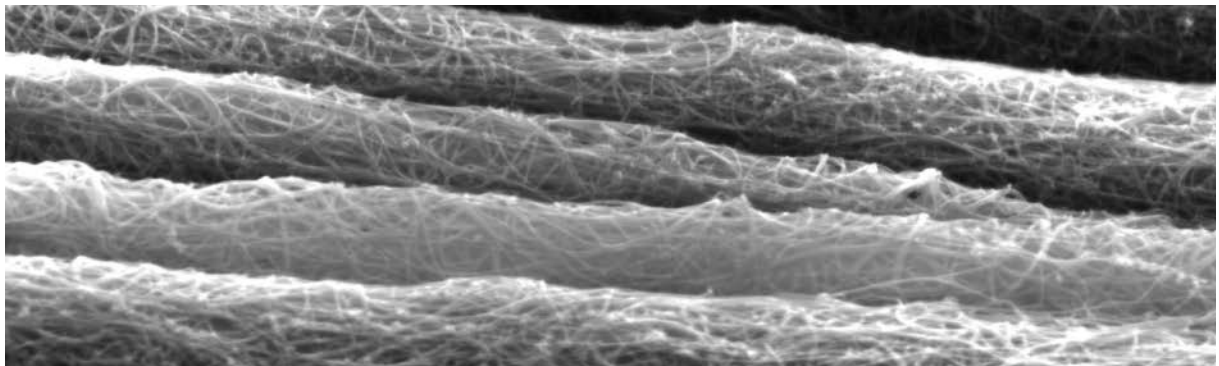
Funding: **Marie Curie Action- CIG, European Union-7th Framework Programme**
Duration: **2013-2017**
Principal Investigator: **Dr. R. Guzmán de Villoria**

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

Funding: **Materials World Network (supported by Spanish Ministry of Economy and Competitiveness and National Science Foundation of the US)**
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**

NETHIPEC "Next generation high performance epoxy-based composites: Green recycling and molecular-level fire retardancy"

Funding: **Spanish Ministry of Economy and Competitiveness**
Duration: **2013-2015**
Principal Investigator: **Dr. D.-Y. Wang**



NANOAL "Nanostructured Al alloys with improved properties"

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

ECOPVC "Eco-friendly fire retardant PVC nanocomposites"

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

HOTNANOMECH "Nanomechanical testing of strong solids at high temperatures"

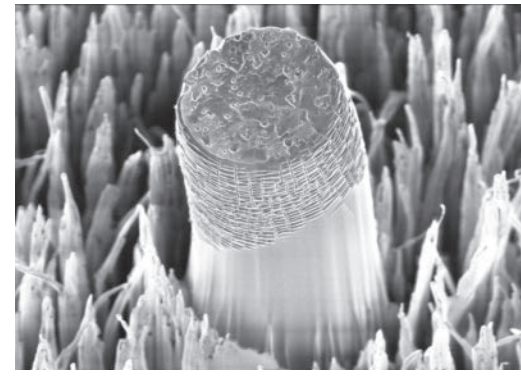
Funding: **Spanish Ministry of Economy and Competitiveness**
Duration: **2013-2016**
Principal Investigator: **Dr. J. M. Molina-Aldareguía**

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**

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

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



MUFIN "Multifunctional fibre nanocomposites"

Funding: **Marie Curie Action-CIG, European Union-7th Framework Programme**
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-CIG, European Union-7th Framework Programme**
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-CIG, European Union-7th Framework Programme**
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: **2012-2014**
Principal Investigator: **Dr. S. Milenkovic**

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

Funding: **AIRBUS OPERATIONS S.L. (Spain)**
Duration: **2012-2015**
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**

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

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

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

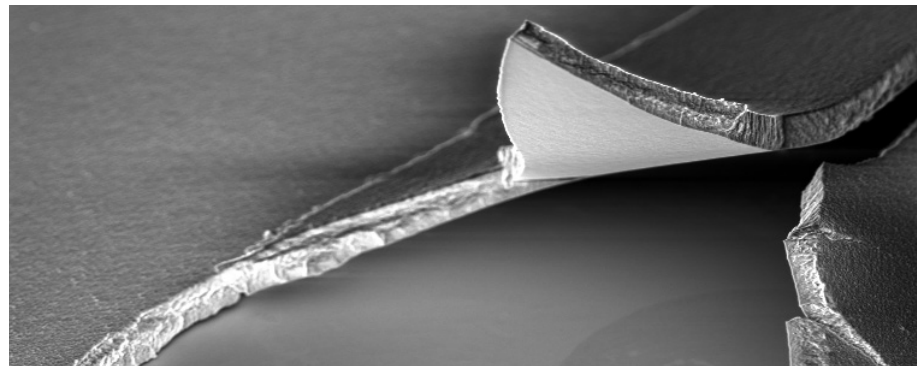
Funding: **NMP, European Union-7th Framework Programme**
Partners: Centre National de la Recherche Scientifique (Coordinator, France), University of Oviedo (Spain), Universidad Politecnica de Madrid (Spain), Ecole des Mines de Paris-ARMINES (France), Czech Technical University in Prague (Czech Republic), 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, European Union-7th Framework Programme**
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, European Union-7th Framework Programme (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: **2011-2014**
Principal Investigator: **Dr. C. González**

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

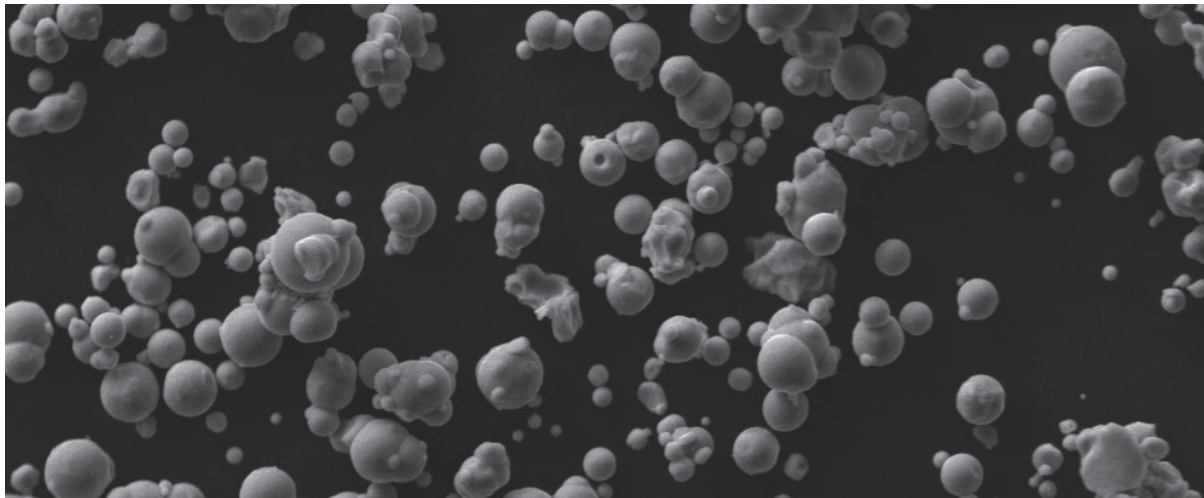
Funding: **Materials World Network (supported by Spanish Ministry of Economy and Competitiveness and National Science Foundation of the US)**
Partners: IMDEA Materials Institute (Spain), Technical University of Madrid (Spain) and Michigan State University (USA).
Duration: **2011-2014**
Principal Investigator: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

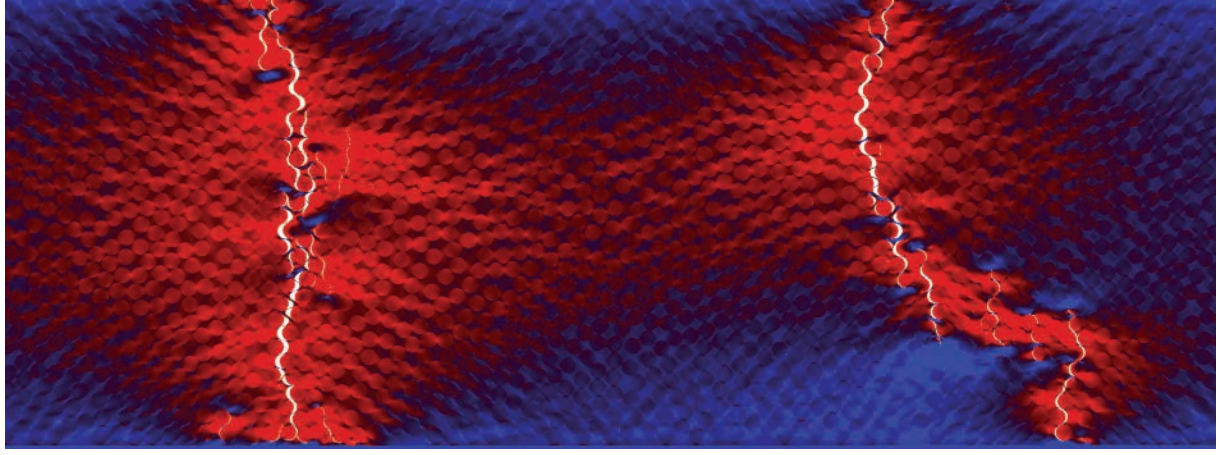
MODELQP "Ginzburg-Landau model for the mixed microstructure in new Q&P steels"

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**

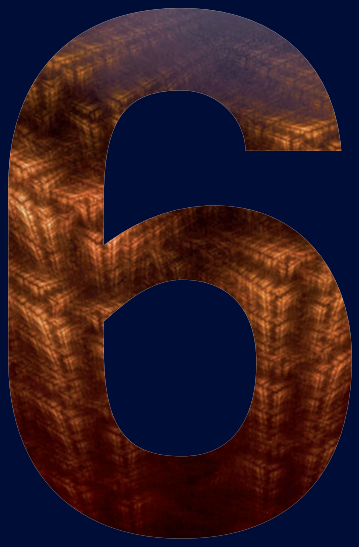
ICE SHEDDING "Design of advanced shields against high-velocity ice impact"

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

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

Funding: **Transport, European Union-7th Framework Programme**
Partners: Consortium of 57 European partners from 18 countries coordinated by AIRBUS OPERATIONS GmbH
Duration: **2008-2016**
Principal Investigator: **Prof. J. LLorca**

dissemination of results



annual report 2014

publications

6.1. Publications

1. J. Terrones, J. A. Elliott, J. J. Vilatela, A. H. Windle, *Electric field-modulated non-ohmic behavior of carbon nanotube fibers in polar liquids*, **ACS Nano 8**, 8497–8504, 2014.

2. R. Sánchez, M. T. Pérez-Prado, J. Segurado, J. Bohlen, I. Gutiérrez-Urrutia, J. LLorca, J. M. Molina-Aldareguia, *Measuring the critical resolved shear stresses in Mg alloys by instrumented nanoindentation*, **Acta Materialia 71**, 283-292, 2014.

3. R. Soler, J. M. Wheeler, H.-J. Chang, J. Segurado, J. Michler, J. LLorca, J. M. Molina-Aldareguia. *Understanding size effects on the strength of single crystals through high temperature micropillar compression*, **Acta Materialia 81**, 50–57, 2014.

4. R. Muñoz, S. Delgado, C. González, B. López-Romano, D.-Y. Wang, J. LLorca, *Modeling lightning impact thermo-mechanical damage in composite materials*, **Applied Composite Materials 21**, 149-164, 2014.

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8. V. Reguero, B. Alemán, B. Mas, J. J. Vilatela, *Controlling carbon nanotube type in macroscopic fibers synthesized by the direct spinning process*, **Chemistry of Materials 26**, 3550–3557, 2014.

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12. J. Vilà, C. González, J. LLorca. *A level set approach for the analysis of flow and compaction during resin infusion in composite materials*, **Composites Part A 67**, 299-307, 2014.

13. A. Salazar, A. Rico, J. Rodríguez, J. Segurado, R. Seltzer, F. Martin de la Escalera, *Fatigue crack growth of SLS polyamide 12: Effect of reinforcement and temperature*, **Composites Part B 59**, 285-292, 2014.

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16. D. A. Vajari, C. González, J. LLorca, B. N. Legarth, *A numerical study of the influence of microvoids in the transverse mechanical response of unidirectional composites*, **Composites Science and Technology 97**, 46-54, 2014.

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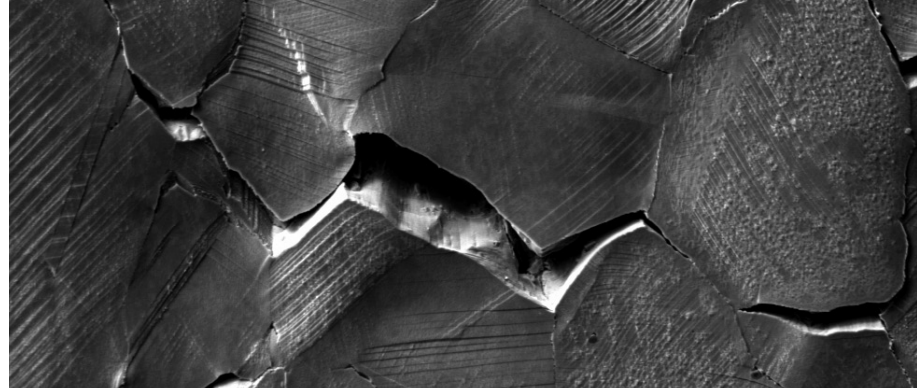

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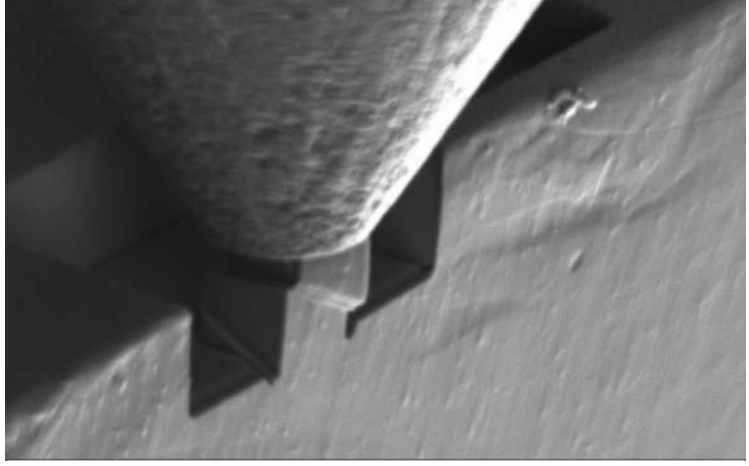

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6.2. Patents

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6.3. License Agreements

1. IMDEA Materials´ **MMonCa** license to QuantumWise A/S (Denmark). Integration of MMonCa into the Atomistix ToolKit package of QuantumWise.

patents

license agreements

6.4. International Conferences

Invited and Plenary talks

1. *"Novel experimental and simulation strategies to determine the single crystal properties of Mg alloys",* J. LLorca, **International Workshop on Modeling and Development of Nanostructured Materials for Biomedical Applications**, Getafe, Spain, February 2014.

2. *"Nanostructuring pure Titanium by field assisted hot pressing of dual phase powder",* B. Srinivasarao, J. M. Torralba, M. A. Jabbari Taleghani, M. T. Pérez-Prado, **International Workshop on Modelling and Development of Nanostructured Materials for Biomedical Applications**, Madrid, Spain, February 2014.

3. *"High temperature mechanical behavior of Al/SiC multilayers",* J. M. Molina-Aldareguia, **The Mineral, Metals and Materials Society – 143rd Annual Meeting and Exhibition (TMS2014)**, San Diego, USA, February 2014.

4. *"Interdiffusion and Atomic Mobility in f.c.c Co-Al Based Ternary Alloys",* Y. Cui, **The Mineral, Metals and Materials Society – 143rd Annual Meeting and Exhibition (TMS2014)**, San Diego, USA, February 2014.

5. *"Physical simulation in metallurgy of aerospace materials",* I. Sabirov, **XIV Jornada de Materiales de la Universidad Carlos III de Madrid**, Madrid, Spain, March 2014.

6. *"Physical simulation at IMDEA Materials Institute",* I. Sabirov, **European Gleeble User Meeting**, Delft, The Netherlands, April 2014.

7. *"Development of processing maps for PM Mg alloys. Mechanical properties",* J. M. Torralba, **5th Academia Day of the Zwick Roell Group**, Móstoles, Spain, April 2014.

8. *"Role of interface structure and crystallography on the mechanical behavior of Cu/Nb multilayers",* J. M. Molina-Aldareguia, **3rd Symposia on Fine Scale Mechanical Characterization (CAMTECIII)**, Cambridge, UK, April 2014.

9. *"Multiscale moldelling of impact in composites: a success story",* J. LLorca, **IUTAM Symposium on Connecting Multiscale Mechanics to Complex Materials Design**, Evanston, USA, May 2014.

10. *"High temperature nanomechanics of nanocomposites",* J. LLorca, **3rd International Conference on Nanomechanics and Nanocomposites**, Hong Kong, China, May 2014.

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12. *"High strength nanostructured Al aloys with multifunctional properties",* I. Sabirov, M. Y. Murashkin, R. Z. Valiev, **XII International Conference on Nanostructured Materials (NANO 2014)**, Moscow, Russia, June 2014.

13. *"Size effects in micropillar compression: the effect of temperature", R. Soler, H.-J. Chang, J. Segurado, J. M. Molina-Aldareguía*, J. LLorca, **IUTAM Symposium on Micromechanics of Defects in Solids**, Seville, Spain, June 2014.

14. *"Size effects during micropillar compression of LiF single crystals: the effect of temperature",* R. Soler, J. Wheeler, J. M. Molina-Aldareguía, H.-J. Chang, J. Segurado, J. Michler, J. LLorca, **17th U.S. National Congress on Theoretical & Applied Mechanics**, East Lansing, USA, June 2014.

15. *"Finite Element Models for Polycrystalline Homogenization*", J. Segurado, **1st International Workshop on Software Solutions for Integrated Computational Materials Engineering (ICMEg)**, Rolduc, Germany, June 2014.

16. *"Stabilization of metastable phases by high pressure torsion",* B. Srinivasarao, A. P. Zhilyaev, T. G. Langdon, M. T. Pérez-Prado, **6th International Conference on Nanomaterials by Severe Plastic Deformation (NANOSPD6)**, Metz, France, June 2014.

17. *"Designing novel materials: From nanoscopic engineering to enhanced macroscopic functionalities",* R. Guzmán de Villoria, **Blue Sky Conference FP7-EYE**, Budapest, Hungary, June 2014.

18. *"New Generation Environmentally Friendly Fire Retardant Epoxy: New Approach to Fire Safety Epoxy Adhesives",* D. Y. Wang, **8th International Conference on Advanced Computational Engineering and Experimenting (ACE-X 2014)**, Paris, France, July, 2014.

19. *"Development of processing routes for fabrication of high strength ultra-fine grained Al alloys",* I. Sabirov, N. A. Enikeev, R. Z. Valiev, M. Y. Murashkin, **The 6th International Conference on Nanomaterials by Severe Plastic Deformation (NanoSPD6)**, Metz, France, July 2014.

20. *"An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests: application to AZ31 and MN11 Mg alloys",* V. Herrera-Solaz, J. Segurado, J. LLorca, **4th International Symposium on Computational Mechanics of Polycrystals**, Düsseldorf, Germany, July 2014.

21. *"An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests by means of computational homogenization",* V. Herrera-Solaz, J. Segurado, J. LLorca, **11th World Congress on Computational Mechanics**, Barcelona, Spain, July 2014.

22. *"Design and development of master alloys for liquid phase sintering",* J. M. Torralba, **ModTech2014 International Conference**, Gliwice, Poland, July 2014.

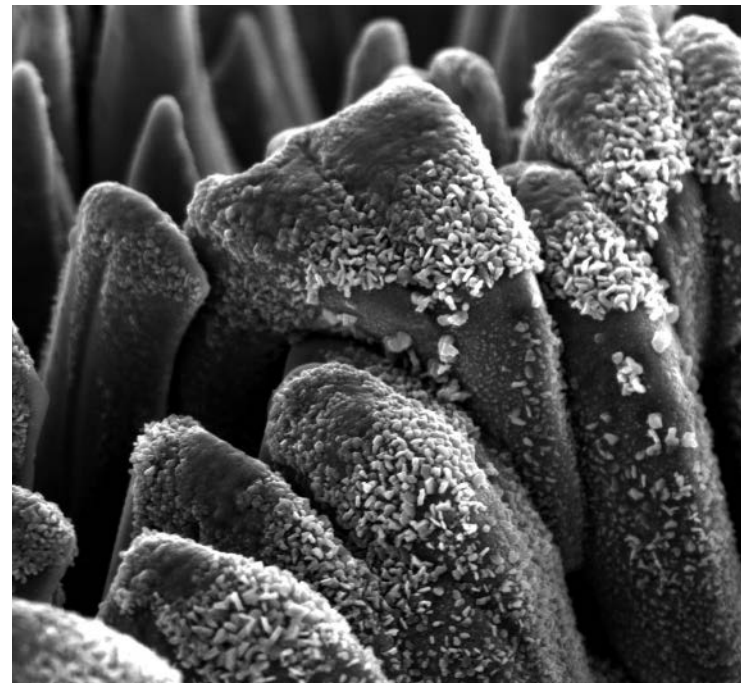
23. *"Mechanical behavior of multilayers as a function of temperature and loading direction",* J. M. Molina-Aldareguia, **Gordon Research Conference: Thin-film and Small Scale Mechanical Behavior**, Waltham, USA, July 2014.

24. *"Physical simulation of solidification: A novel tool for accelerated screening of solidification-microstructure relationships",* S. Milenkovic, M. Rahimian, I. Sabirov, **4th International Conference on Advances in Solidification Processes (ICASP 4)**, Windsor, UK, July 2014.

25. *"Development of novel milled Co- base superalloys consolidated by Field-Assisted Hot Pressing",* J. M. Torralba, **International Conference on Sintering**, Dresden, Germany, August 2014.

26. *"A fully Lagrangian method for fluid/solid interaction",* I. Romero, M. Urrecha, **Symposium on Innovative numerical approaches for materials and structures in multi-field and multi-scale problems**, Attendorn, Germany, September 2014.

27. *"Fracture properties of quenched and partitioned steels",* I. de Diego, D. De Knijf, R. Petrov, J. M. Molina-Aldareguia, I. Sabirov, **European Workshop on Advanced Steels: Challenges in Steel Science and Technology**, Madrid, Spain, September 2014.



28. *"Understanding the Contribution of the Microstructure in the Fracture Behaviour of Sintered Steels*", J. M. Torralba, **Euro PM 2014 Congress & Exhibition**, Salzburg, Austria, September 2014.

29. *"Development of Zircon by Powder Injection Moulding*", J. M. Torralba, **The Third Serbian Ceramic Society Conference »Advanced Ceramics and Application**, Belgrade, Serbia, September 2014.

30. *"Multifunctional self-organized nanowires and nanowire arrays",* S. Milenkovic, A. W Hassel, **Symposium on New Frontiers in Multifunctional Material Science and Processing**, Belgrade, Serbia, September 2014.

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32. *"Recent developments of computational and experimental micromechanics of composites",* C. González, **XXIV International Workshop on Computational Micromechanics of Materials**, Getafe, Spain, October 2014.

33. *"Effect of indentation size on the nucleation and propagation of tensile twinning in pure magnesium single crystals",* J. M. Molina-Aldareguia, R. Sanchez, M. T. Pérez-Prado, J. Segurado, **XXIV International Workshop on Computational Micromechanics of Materials**, Getafe, Spain, October 2014.

34. *"Development of Novel Fire Retardant Textiles and New Generation High Performance Fire Retardant Polymer Composites",* D. Y. Wang, **2014 Leadership Symposium of Advanced Textile**, Beijing, China, October 2014.

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36. *"Modeling of a Ni-based superalloy: from micro-pillar compression tests to polycrystalline models",* J. Segurado, A. Cruzado, H.-J. Chang, B. Gan, S. Milenkovic, J. M. Molina-Aldareguía, J. LLorca, **7th International Conference on Multiscale Materials Modeling**, Berkeley, USA, October 2014.

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38. *"Influence of grain boundaries on slip activity and twin propagation in magnesium",* M. T. Pérez-Prado, **The 2nd International Symposium on Long Period Stacking Order Structure and its Related Materials (LPSO 2014)**, Kumamoto, Japan, October 2014.

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40. *"Understanding the fracture behaviour of PM steels through in situ tests",* J. M. Torralba, **Höganäs Powder Science Symposium**, Örenäs Slott, Sweden, November 2014.

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Regular Contributions

1. *"Advanced simulation of low-velocity impact on fibre reinforced laminates",* C. S. Lopes, S. Sádaba, P. P. Camanho, C. González, **4th International Conference on Impact Loading of Lightweight Structures**, Cape Town, South Africa, January 2014.

2. *"Investigation of void growth in single crystals by using Discrete (MD) and continuum (DD) simulation",* H.-J. Chang, J. Segurado, O. Rodríguez, J. LLorca, **International Workshop on Modeling and Development of Nanostructured Materials for Biomedical Applications**, Getafe, Spain, February 2014.

3. *"Multiscale modeling of a small punch test on hydrostatically extruded titanium*", A. Ridruejo, J. Segurado, I. Sabirov, J. LLorca, **International Workshop on Modeling and Development of Nanostructured Materials for Biomedical Applications**, Getafe, Spain, February 2014.

4. *"Simulation of temperature effect on the deformation of nano-Ti by computational homogenization",* J. Segurado, I. Sabirov, D. Rodriguez, **International Workshop on Modeling and Development of Nanostructured Materials for Biomedical Applications**, Getafe, Spain, February 2014.

5. *"Modeling the high temperature deformation of Al/SiC nanolaminates*", N. Chawla, J. M. Molina-Aldareguia, S. Lotfian, C. Mayer, J. LLorca, A. Misra, **The Mineral, Metals and Materials Society – 143rd Annual Meeting and Exhibition (TMS2014)**, San Diego, USA, February 2014.

6. *"High temperature deformation of PVD and ARB Cu/Nb multilayers*", J. M. Molina-Aldareguia, M. Monclús, I. Beyerlein, N. Mara, T. Polcar, J. LLorca, **The Mineral, Metals and Materials Society – 143rd Annual Meeting and Exhibition (TMS2014)**, San Diego, USA, February 2014.

7. *"Measuring the critical resolved shear stress in magnesium alloys by instrumented nanoindentation*", J. M. Molina-Aldareguía, R. Sánchez, M.T. Pérez-Prado, J. Segurado, J. LLorca, **The Mineral, Metals and Materials Society – 143rd Annual Meeting and Exhibition (TMS2014)**, San Diego, USA, February, 2014.

8. *"Versatile aligned eutectics: from high temperature structural materials to functional nanodevices*", S. Milenkovic, A. W. Hassel, **The Mineral, Metals and Materials Society – 143rd Annual Meeting and Exhibition (TMS2014)**, San Diego, USA, February 2014.

9. *"Photocatalytic water splitting using CNT-inorganic hybrid material",* A. Moya, J. J. Vilatela, **European Hydrogen Energy Conference, EHEC 2014**, Seville, Spain, March 2014.

10. *"Diffusion and Mobility in Co-Al-based Ternary Alloys: Diffusion Couple Experiment and Assessment",* Y. Cui, **NIST Diffusion Workshop**, Gaithersburg, USA, April 2014.

11. *"Lattice Kinetic Monte Carlo modeling of solid phase epitaxial regrowth for silicon and germanium materials*", I. Martin-Bragado, J. L. Gomez-Selles, B. Sklenard, **European MRS (E-MRS 2014)**, Lille, France, May 2014.

12. *"Metal Organic Frameworks incorporated into electrospun polylactic acid show remarkable antimicrobial effects",* J. Quirós, S. Aguado, K. Boltes, R. Guzman de Villoria, J. J. Vilatela, R. Rosal, **Baku World Forum of Young Scientists 2014**, Baku, Azerbaijan, May 2014.

13. *"Effect of solidification parameters on the dendrite arm spacing in MAR M-247",* S. Milenkovic, M. Rahimian, I. Sabirov. **EUROSUPERALLOYS 2014**, Giens, France, May 2014.

14. *"On the use of dic-3D to determine the permeability tensor and compaction law of fabric by VARTM",* J. Vila, C. González, J. LLorca, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

15. *"Modelization of advanced nonwoven fabrics subjected to tensile loads*", F. Martínez, A. Ridruejo, F. Gálvez, C. González, J. LLorca, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

16. *"Thermo-mechanical damage due to lightning impact in carbon/epoxy composites: experiments and simulations",* C. González, S. Delgado, F. Sket, J. LLorca, D. Y. Wang, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

17. *"Combined multi-scale simulations In fiber-reinforced composites",* F. Naya, C. González, C. Lopes, S. Van Der Veen, J. LLorca, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

18. *"Analisys of transverse cracking in unidirectional composite plies by means of computational micromechanics",* D. Mora, C. González, C. Lopes, J. LLorca, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

19. *"Mechanical behaviour of hybrid 3D woven composites under static and impact loads",* R. Muñoz, F. Martínez-Hergueta, R. Seltzer, C. González, J. LLorca, **16th European European Conference on Composite Materials**, Seville, Spain, June 2014.

20. *"Electric curing of nanocarbon/epoxy adhesives for composite repair",* A. Monreal-Bernal, J. J. Vilatela, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

21. *"Production and properties of composites based of carbon nanotube fibre",* B. Mas, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

22. *"Click chemistry: towards self-healing polymer composite",* H. Yue, J. J. Vilatela, J. P. Fernández-Blázquez, **16th European Conference on Composite Materials**, Seville, Spain, June 2014.

23. *"New findings on fire retardant epoxy nanocomposites",* D. Y. Wang, **3rd International Symposium on Flame-Retardant Materials & Technologies (ISFRMT 2014)**, Hefei, China, June 2014.

24. *"Atomistic simulations of solid-phase epitaxy regrowth of silicon amorphized via ion implantation",* M. Prieto-Depedro, I. Romero, I. Martin-Bragado, **Computer Simulation of Radiation Effects in Solids (COSIRES 2014)**, Alicante, Spain, June 2014.

25. *"Parallelism in object Kinetic Monte Carlo: implementation and results for lattice and off-lattice approaches",* I. Martin-Bragado, J. Abujas, P. L. Galindo, J. Pizarro, **Computer Simulation of Radiation Effects in Solids (COSIRES 2014)**, Alicante, Spain, June 2014.

26. *"Microstructural evolution in BCC iron under irradiation: Impact of carbon",* D. Terentyev, I. Martin-Bragado, Y. Osetsky, A. Serra, **Computer Simulation of Radiation Effects in Solids (COSIRES 2014)**, Alicante, Spain, June 2014.

27. *"Ion-beam induced damage in Ge: An atomistic approach",* J. L. Gomez-Selles, B. Sklenard, I. Martin-Bragado, **Computer Simulation of Radiation Effects in Solids (COSIRES 2014)**, Alicante, Spain, June 2014.

28. *"X-Ray computed tomography analysis of deformation and damage mechanisms of fiber-reinfoced composites in shear",* F. Sket, A. Enfedaque, C. Alton, C. Gonzalez, J. M. Molina-Aldareguía, J. LLorca, **17th U.S. National Congress on Theoretical & Applied Mechanics**, Michigan, USA, June 2014.

29. *"An inverse optimization strategy to obtain single crystal mechanical properties from polycrystal tests: application to Mg alloys",* V. Herrera-Solaz, J. Segurado, J. LLorca, **17th U.S. National Congress on Theoretical & Applied Mechanics**, Michigan, USA, June 2014.

30. *"In situ study of tension and compression deformation behavior of rare-earth (Nd) containing extruded Mg-1Mn (wt%) alloys",* A. Chakkedath, J. Bohlen, S. Yi, D. Letzig, Z. Chen, C. J. Boehlert, M. T. Pérez-Prado, J. LLorca, **17th U.S. National Congress on Theoretical & Applied Mechanics**, Michigan, USA, June 2014.

31. *"Optimización de feedstocks ecológicos basados en circón para moldeo por inyección",* C. Abajo, A. Jiménez-Morales, J. M. Torralba, **V Congreso Nacional Materiales**, Barcelona, Spain, June 2014.

32. *"Obtención de materiales magnéticos blandos fabricados por moldeo por inyección (MIM) para el diseño de imanes",* A. Páez-Pavón, A. Jiménez-Morales, T. Santos, L. Quintino, J. M. Torralba, **V Congreso Nacional Materiales**, Barcelona, Spain, June 2014.

33. *"Mechanical behavior at different temperatures and strain rates of an extruded magnesium-manganese alloy containing neodymiu",* P. Hidalgo-Manrique, V. Herrera-Solaz, J. Segurado, J. LLorca, F. Gálvez, O.A. Ruano, S.B. Yi, J. Bohlen, D. Letzig, M. T. Pérez-Prado, **IMA's 71st Annual World Magnesium Conference**, Munich, Germany, June 2014.

34. *"Landau model of martensite in steels and shape memory alloys",* Y. Cui, G. Xu, D-W Lee, **1st International Workshop on Software Solutions for Integrated Computational Materials Engineering**, Aachen/Rolduc, Germany, June 2014.

35. *"Exploring the formation mechanism of solidified eutectic structures in ternary NiAl-based alloys by thermodynamic phase field modeling",* B. Tang, S. Milenkovic, Y. Cui, J. Li, **1st International Workshop on Software Solutions for Integrated Computational Materials Engineering**, Aachen/Rolduc, Germany, June 2014.

36. *"Integrated Landau model for martensite in steels and shape memory alloys",* Y. Cui, G. Xu, D-W Lee, **CALPHAD XLIII**, Changsha, China, June 2014.

37. *"A stable X-FEM in cohesive transition from closed to open crack",* S. Sadaba, I. Romero, C. Gonzalez, J. LLorca, **11th World Congress on Computational Mechanics**, Barcelona, Spain, July 2014.

38. *"Energy-consistent time integration for nonlinear viscoelasticity",* S. Conde, J. C. García, I. Romero, **11th World Congress on Computational Mechanics**, Barcelona, Spain, July 2014.

39. *"Some numerical aspects of finite element models for polycrystalline homogenization",* D. Rodriguez, I. Romero, J. Segurado, **11th World Congress on Computational Mechanics**, Barcelona, Spain, July 2014.

40. *"Lattice Kinetic Monte Carlo simulations of epitaxial processes for Si and Ge materials",* I. Martin-Bragado, **CMOS-Emerging Technologies Research**, Grenoble, France, July 2014.

41. *"Introduction to Kinetic Monte Carlo simulations using MMonCa". I. Martín-Bragado,* ***International Workshop on Advanced Nuclear Materials****, Gijón, Spain, July 2014.*

42. *"Micro- and nano-mechanical testing"*, M. A. Monclus, **International Workshop on Advanced Nuclear Materials**, Gijon, Spain, July 2014.

43. *"Modeling of a Ni-based superalloy: From micropillar compression to polycrystalline models",* J. Segurado, A. Cruzado, B. Gan, S. Milenkovic, J. M. Molina-Aldareguia, J. LLorca, **4th International symposium on Computational Mechanics of Polycrystals cmcn 2014**, Düsseldorf, Germany, July 2014.

44. *"Outstanding antibacterial activity of cobalt imidazolate metal-organic framework incorporated into electrospun fibers",* J. Quirós, S. Aguado, K.Boltes, R. Guzman de Villoria, J. J. Vilatela, R. Rosal, **ANQUE 2014 Conference**, Seville, Spain, July 2014.

45. *"Physical simulation of solidification: A novel tool for accelerated screening of solidification-microstructure relationships",* S. Milenkovic, M. Rahimian, I. Sabirov, 4th Intern. **Conference on Advances in Solidification Processes (ICASP 4)**, Windsor, UK, July 2014.

46. *"Atomistic simulation of diffusion in alloys using non-lattice Kinetic Monte Carlo methods",* I. Dopico, P. Castrillo, I. Martin-Bragado, **International Conference on Diffusion in Materials (DIMAT 2014)**, , Münster, Germany, August 2014.

47. *"Modeling of a Ni-based superalloy: From micropillar compression to polycrystalline models",* J. Segurado, A. Cruzado, B. Gan, S. Milenkovic, J. M. Molina-Aldareguia, J. LLorca, **14th European Mechanics of Materials Conference, EMMC-14**, Gothenburg, Sweden, August 2014.

48. *"Synthesis of kilometres of continuous macroscopic fibres with controlled type of carbon nanotube",* J. J. Vilatela, **Carbonhagen 2014**, Copenhagen, Denmark, August 2014.

49. *"Multiscale Simulation Strategy for Low-Velocity Impact on FRP",* C. S. Lopes, F. Naya, S. Sádaba, C. González, **American Society for Composites (ASC) 29th Technical Conference & 16th US-Japan Conference on Composite Materials**, La Jolla, USA, September 2014.

50. *"Multiscale simulation strategy for low-velocity impact on FRP",* C. S. Lopes, F. Naya, C. González, P. P. Camanho, **2nd International Journal of Structural Integrity Conference**, Funchal, Portugal, September 2014.

51. *"Mechanisms of the phase separation of nonstoichiometric Si oxide films: What can one learn from thermodynamics?",* A. Sarikov, **4th International Conference "Nanomaterials: Applications and Properties-2014 (NAP-2014)**, Lviv, Ukraine, September 2014.

52. *"Fracture behaviour of quenched and partitioned steels",* I. de Diego, D. De Knijf, J. M. Molina-Aldareguia, I. Sabirov, C. Fojer, R. Petrov, **International Conference on Materials Science and Engineering**, Darmstadt, Germany, September 2014.

53. *"Development of Fe-based soft magnetic alloys by Metal Injection Molding (MIM)",* A. Páez-Pavón, A. Jiménez-Morales, T. Santos, L. Quintino, J. M. Torralba, **EuroPM Congress 2014**, Saltzburg, Austria, September 2014.

54. *"Master alloy compositions for tailoring liquid phases in lean steels",* E. Bernardo, R. Oro, M. Campos, J. M. Torralba, **EuroPM Congress 2014**, Saltzburg, Austria, September 2014.

55. *"Controlled type of CNT in macroscopic fibre synthesised by the direct spinning method",* V. Reguero, J. J. Vilatela**, International Conference on Carbon and Diamond Materials**, Madrid, Spain, September 2014.

56. *"Efecto de las adiciones de Nd en la microestructura, textura y propiedades mecánicas de aleaciones de Mg",* P. Hidalgo-Manrique, V. Herrera-Solaz, J. Segurado, J. LLorca, F. Gálvez, O. A. Ruano, S. B. Yi, J. Bohlen, D. Letzig, M. T. Pérez-Prado, **XIV Congreso Nacional de Propiedades Mecánicas de Sólidos (PMS 2014)**, Linares, Spain, September 2014.

57. *"Study of the dominant deformation mechanisms in pure magnesium by in situ testing and trace analysis",* C. M. Cepeda-Jiménez, J. M. Molina-Aldareguia, I. Gutiérrez-Urrutia, M. T. Pérez-Prado, **35th Risø International Symposium on Materials Science**, Roskilde, Denmark, September 2014.

58. *"Microstructure evolution and mechanical behaviour of as-cast, heat treated and directionally solidified Fe-15Al-10Nb alloys",* S. Milenkovic, G. Yang, **13th International Symposium on Advanced Physics of Metals (ISPMA 13)**, Prague, Czech Republic, September 2014.

59. *"Characterization of the deformation micro-*

mechanisms and texture evolution of needle-punched nonwoven fabrics: an experimental and numerical study", F. Martínez-Hergueta, A. Ridruejo, F. Gálvez, C. González, J. LLorca, **XXIV International Workshop on Computational Micromechanics of Materials**, Getafe, Spain, October 2014.

60. *"Non-circular cross section carbon fibers",* M. Herráez, C. González, C. S.Lopes, R. Guzmán de Villoria, **XXIV International Workshop on Computational Micromechanics of Materials**, Getafe, Spain, October 2014.

61. *"Multiscale modeling of grain boundary motion coupled to shear deformation",* I. Martín-Bragado , M. Prieto, J. Segurado, **XXIV International Workshop on Computational Micromechanics of Materials**, Getafe, Spain, October, 2014.

62. *"Size effects during micropillar compression: the effect of temperature and lattice resistance*", H.-J. Chang, R. Soler, J. Segurado, J. M. Molina-Aldareguía, J. LLorca, **XXIV International Workshop on Computational Mechanics of Materials**, Getafe, Spain, October 2014.

63. *"Crystal plasticity modelling of polycrystalline IN718*", J. Segurado, A. Cruzado, B. Gan, J. M. Molina-Aldareguia, J. LLorca, **XXIV International Workshop on Computational Mechanics of Materials**, Getafe, Spain, October 2014.

64. *"Multiscale modeling of deformation in hydrostatically extruded Ti",* A. Ridruejo, J. Segurado, I. Sabirov, J. LLorca, **XXIV International Workshop on Computational Mechanics of Materials**, Getafe, Spain, October 2014.

65. *"Effect of indentation size on the nucleation and propagation of tensile twinning in pure magnesium single crystals",* J. M. Molina-Aldareguia, R. Sanchez, M. T. Pérez-Prado, J. Segurado, **XXIV International Workshop on Computational Micromechanics of Materials**, Getafe, Spain, October 2014.

66. *"Effect of temperature on the critical resolved shear stress of MN11 magnesium alloy",* V. Herrera-Solaz, P. Hidalgo-Manrique, M. T. Pérez-Prado, J. LLorca, J. Segurado, **XXIV International Workshop on Computational Micromechanics of Materials**, Getafe, Spain, October 2014.

67. *"Layer by layer assembly of multilayered coating made from natural polysaccharides for improving fire retardancy of poly(ethylene terephthalate*)", D. Y. Wang, **Workshop of Characterization of Flame Retardant Textile and Related Materials**, Dubrovnik, Croatia, October 2014

68. *"Modelling of damage accumulation and dissolution mechanisms in ion-implanted Ge",* J. L. Gomez-Selles, A. Claverie, F. Benistant, I. Martin-Bragado, **IEEE Nanotechnology Materials and Devices (IEEE-NMDC 2014) Conference**, Aci Castello, Italy, October 2014.

69. *"Combined molecular dynamics and Object Kinetic Monte Carlo simulations of ion implantation in Fe thin films",* M. J. Aliaga, I. Martin-Bragado, M. J. Caturla, **7th International Conference on Multiscale Materials Modeling**, Berkeley, California, October 2014.

70. *"A 3D dislocation dynamics analysis of the development of size effects at high temperature during micropillar compression ol LiF [111] single crystals",* H.-J. Chang, J. Segurado, R. Soler, J. M. Molina-Aldareguía, J. LLorca, **7th International Conference on Multiscale Materials Modeling**, Berkeley, USA, October 2014.

71. *"Amorphous Carbon Films Synthesized by Chemical Vapor Deposition Process",* P. Romero, R. Guzman de Villoria, **XXX Trobades Cientifiques de la Mediterrania, Graphene and Related Materials**, Menorca, Spain, October 2014.

72. "*Microstructure and mechanical properties of PVD Cu/W and Zr/Nb nanoscale multilayers*", M. A. Monclus, **14th European Nanomechanical User Group Meeting,** Madrid, Spain, November 2014.

73. *"Damage and defects assessment in composite materials using X-ray Computed Tomography*", F. Sket, J. M. Molina-Aldareguía, C. González, J. LLorca, **6th Symposium for non-destructive testing in aerospace**, Madrid, Spain, November 2014.

74. *"Synthesis of vertically aligned carbon nanotubes and nanocrystalline A-C film on stainless steel by chemical vapour deposition",* P. Romero, R. De Oro, M. Campos, J. M. Torralba, R. Guzman de Villoria, **Materials Research Society Fall Meeting & Exhibit**, Boston, USA, December 2014.

membership in organizing committees

Membership in Organizing Committees

1. **USACM/IUTAM International Symposium on Connecting Multiscale Mechanics to Complex Material Design.** J. LLorca. (Symposium Co-Organizer). Evanston, USA, May 2014.

2. **Computer Simulation of Radiation Effects in Solids, COSIRES 2014.** I. Martin-Bragado. (Member of the Local Organizing Committee). Alicante, Spain, June 2014.

3. **XII International Conference on Nanostructured Materials, NANO 2014.** I. Sabirov. (Member of section program board, Bulk Metallic Nanomaterials). Moscow, Russia, July 2014.

4. **International Symposium on Integrated Computational Materials Engineering at the 11th World Congress on Computational Mechanics, WCCM XI,** J. LLorca. (Symposium Co-Organizer). Barcelona, Spain, July 2014

5. **Second International Conference of Young Researchers on Advanced Materials, IUMRS-ICYRAM.** I. Sabirov. (Symposium Co-Organizer, Light Alloys and Metal-based Composites). Haikou, China, October 2014.

6. **13th International Workshop on Stress-Induced Phenomena in Microelectronics.** J. M. Molina-Aldareguia (Scientific Committee). Austin, Texas. October 2014.

7. **The 2nd International Symposium on Long Period Stacking Order Structure and its Related Materials, LPSO 2014,** M. T. Pérez-Prado (Member of the Steering Committee), Kumamoto, Japan, October 2014.

8. **Advanced Materials and Processing Technologies, AMPT'2014,** J. M. Torralba (Steering Committee), Dubai, United Arabs Emirates, November 2014.

9. **6th Symposium for non-destructive testing in aerospace, NDT in Aerospace,** F. Sket (Organising Committee). Madrid, Spain, November 2014.

6.5. Hosting and Organization of International Workshops

international workshops

Two international workshops (devoted to modelling and development of nanostructured materials for biomedical applications and Computational Mechanics of Materials) were held at IMDEA Materials Institute in 2014, taking advantage of the facilities available in our building. Over 100 researchers attended these events, enhancing the international visibility of our activities.

1. **International workshop on modeling and development of nanostructured materials for biomedical applications,** I. Sabirov, L. Mishnaevsky, E. Levashov and J. Segurado (Organizers), February 2014.

2. **24th International Workshop on Computational Mechanics of Materials**, J. Segurado, J. LLorca and S. Schmauder (Organizers), October 2014

Figure 5. Conference facilities at IMDEA Materials Institute. Main hall during a poster session

Figure 6. IMDEA Materials Institute Auditorium

6.6. Invited Seminars and Lectures

1. *"A model for the multiscale simulation of alloys at finite temperature"*. I. Romero, **University of A Coruña**, A Coruña, Spain, January 2014.

2. *"Multiscale Modelling Of Composites: Towards Virtual Testing and Design"*. C. S. Lopes, **University of Manchester**, Manchester, UK, February 2014.

3. *"Advanced fire retardant textiles"*. D. Y. Wang, **Jilin Chemical Fiber Group Company**, Jilin, China, February 2014.

4. *"New generation fire safe polymeric materials"*. D. Y. Wang, **Anhui University of Science and Technology**, Huainan, China, March 2014.

5. *"Experimental & computational micromechanics: exploring the mechanical properties at the nm-μm scale"*. J. LLorca. Materials and Structures Branch, **ONERA**, Chatillon, France, March 2014.

6. *"High Throughput Diffusion Research for Novel Rare Metals"*, Y. Cui, School of Materials Science and Engineering, **Northwestern Polytechnical University**, Xi'an, China, March 2014.

7. *"Materiales por ordenador, simulando el futuro"*. I. Martín-Bragado, **Complutense University of Madrid**, Madrid, Spain, May 2014

8. *"High temperature nanomechanics"*. J. LLorca. **Korea Institute of Science and Technology**, Seoul, South Korea, May 2014.

9. *"High temperature nanomechanics"*. J. LLorca. Department of Materials Science and Engineering, **Seoul National University**, Seoul, South Korea, May 2014.

10. *"Multiscale modelling of nanoengineered composites: a roadmap towards virtual testing"*. J. LLorca. **Korea Institute of Materials Science**, Changwon, South Korea, May 2014.

11. *"Multifunctional nanomaterials and high performance fire retardant polymer nanocomposites"*. D. Y. Wang, **Southwest University of Science and Technology**, Mianyang, China, June 2014.

12. *"Analysis of mechanical properties in a quenched and partitioned steel"*. I. Sabirov, **OCAS - ArcelorMittal Global R&D Gent**, Gent, Belgium, June 2014.

13. *"Large-scale synthesis, properties and application of self-organized metallic nanowires and nanowire arrays"*, S. Milenkovic. **Serbian Academia of Sciences and Arts**, Belgrade, Serbia, June 2014.

14. *"Development of advanced PM materials"*, J. M. Torralba, **University of Erlangen-Nürnberg**, Erlangen, July 2014

15. *"Fluid/solid interaction with a Lagrangian meshless method"*. I. Romero, Department of Civil Engineering, **Stuttgart University**, Stuttgart, Germany, August 2014.

16. *"Multiscale Modelling Of Composites: Towards Virtual Testing and Design"*. C. S. Lopes, **Fokker Aerostructures**, Papendrecht, The Netherlands, August 2014.

17. *"Integrated Landau Model for Martensite in Steels and Shape Memory Alloys"*, Y. Cui, State Key Lab of Metal Matrix Composites, **Shanghai Jiaotong University**, Shanghai, China, August 2014.

18. *"New generation Fire Retardant Polymer Nanocomposites"*. D. Y. Wang, Institute of Chemistry, **The Chinese Academy of Sciences**, Beijing, China, October 2014,

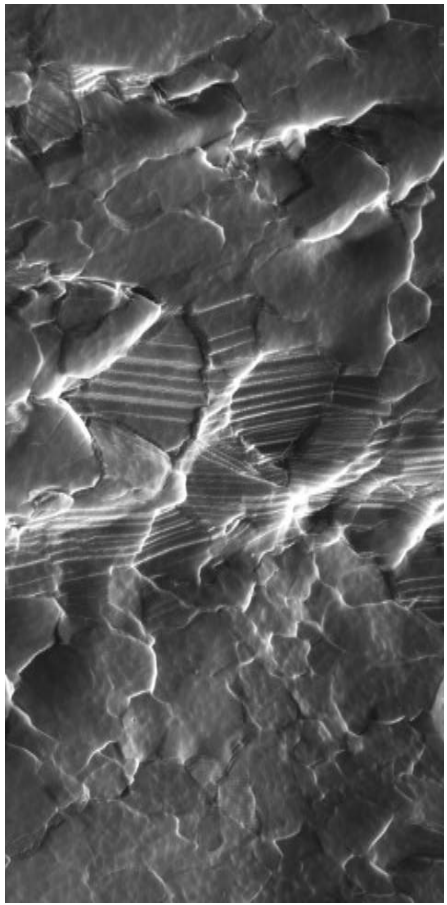
19. *"High strength nanostructured Al alloys with enhanced electrical conductivity"*. I. Sabirov. **Shanghai Jiao Tong University**, Shanghai, China, October 2014.

20. *"Towards the next generation of composite materials"*. J. LLorca, Gill Composites Center, **University of Southern California**, Los Angeles, California, October 2014.

21. *"Growth and properties of self-organized metallic nanowires and nanowire arrays"*, S. Milenkovic. Faculty of Technology and Metallurgy, **University of Belgrade**, Serbia, October 2014.

22. *"Kinetic Monte Carlo: An introduction"*. I. Martín-Bragado, **Complutense University of Madrid**, Madrid, Spain, November 2014

23. *"Multifunctional materials based on continuous macroscopic fibres of carbon nanotubes combined with polymers and semiconductors"*. J. Vilatela. Centro de Investigación en Dispositivos Semiconductores, **Benemérita Autonomous University of Puebla (BUAP)**, Puebla, Mexico, December 2014.



6.7. Seminars

1. *"Nano-mechanics towards advanced materials"*, **Dr. In-Suk Choi** (from Korea Institute of Science and Technology, Seoul, South Korea). February 2014.

2. *"Spontaneous adiabatic shear localization in electromagnetically collapsing cylinders"*, **Prof. Daniel Rittel** (from Technion, Haifa, Israel). April 2014.

3. *"Modeling fatigue properties in textile-reinforced composites"*, **Dr. Jian Xu** (from Compositence GmbH, Germany). April 2014.

4. *"Dislocation microstructure studies in ceramics. Dissociation and plasticity"*, **Dr. Miguel Castillo Rodríguez** (from Materials Science Institute of Seville-CSIC, Spain). April 2014.

5. *"Industrial development and industrial processing of FeAl alloys"*, **Dr. Martin Palm** (from Max-Planck-Institut für Eisenforschung GmbH). May 2014.

6. *"Monte Carlo modeling of nanodevices for semiconductor and biological applications"*, **Dr. Jean-Francois Millithaler** (from Université Montpellier 2 Sciences et Techniques, France). June 2014.

7. *"Hierarchical composite materials: routes and applications"*, **Dr. Tomi Herceg** (from Imperial College, UK). July 2014.

8. *"Introducing ductility to composite materials"*, **Dr. Meisan Jalalvand** (from University of Bristol, UK). July 2014.

9. *"Sustainable composites for commercial aviation and building infrastructure sectors"*, **Prof. Debes Bhattacharyya** (from University of Auckland, New Zealand). July 2014.

10. *"High temperature single crystal creep deformation mechanisms of new L12-containing Co-base superalloys"*, **Dr. Michael Titus** (from University of California, USA). August 2014.

11. *"Hybrid-interface based Future Materials"*, **Prof. Kwangho Kim** (from Pusan National University). September 2014.

12. *"Composite materials' activity of South Ural State University (Russia): past and future of structural and ballistic applications"*, **Prof. Sergei B. Sapozhnikov** (from South Ural State University). September 2014.

13. *"IMDEA Materials Research Initiation Fellowships 2014"*, **Sergio García, Álvaro Menduiña, Bogdan Nedelcu and Rafael Sancho** (2014 research initiation fellows). September 2014.

14. "*Microstructure-sensitive fatigue modeling"*, **Prof. David L. McDowell** (from Woodruff School of Mechanical Engineering / Georgia Institute of Technology). November 2014.

15. *"Recent advances in modelling of metal machining processes"*, **Dr. Pedro Arrazola** (from Mondragón University). November 2014.

16. *"Studies of polymer deformation by 2D X-ray diffraction"*, **Prof. Ernesto Pérez** (from Polymer Science and Technology CSIC). November 2014.

17. *"High-strain composite materials and their application to deployable space structures"*, **Dr. Ignacio Maqueda** (from California Institute of Technology). November 2014.

18. *"Trends and advances in powder metallurgy steels for structural applications"*, **Dr. Dimitris Chasoglou** (from Höganäs AB). December 2014.

19. "Beyond graphene: The amazing world of layered transititon metal dichalcogenides", **Dr. Humberto Terrones** (from Rensselaer Poyltechnic Institute). December 2014.

6.8 Fellowships

1. AMAROUT EUROPE Programmes (I and II), Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
- Call 2014: **Dr. C. Coluccini, Dr. E. Bonifaz, Dr. A. Sarikov, Dr. V. Babu, Dr. J. Xu, Dr. J-H Zhang, Dr. D. González, Dr. S. Haldar, Dr. J. P. Balbuena**
- Call 2013: **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 2013: **Dr. C. S. Lopes, Dr. M. Haranczyk**
- 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. *Postdoctoral Fellowship Programmes, Spanish Ministry of Economy and Competitiveness*
- Call 2013: **Dr. F. Sket**
- 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 2014: **C. Wang, Q. Liu**
- Call 2013: **Y. Pang, Y. Lingwei**
- Call 2012: **Y. Chen, X. Zhao**
- Call 2011: **G. Xu, H. Yue**

fellowships

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 2013: **R. Sánchez**
· Call 2012: **F. Martínez-Hergueta**

7. Predoctoral Fellowships Programmes, Spanish Ministry of Economy and Competitiveness
· Call 2013: **A. Palomares**

6.9. Awards

1. Science and Technology Advisor of Shenyang City, China,
· **Dr. D. Y. Wang**

2. Adjunct Professorship of South China University of Technology
· **Dr. D. Y. Wang**

3. Young Researcher Award for outstanding contribution to research on nano severe plastic deformation, NanoSPD6 Conference.
· **Dr. I. Sabirov**

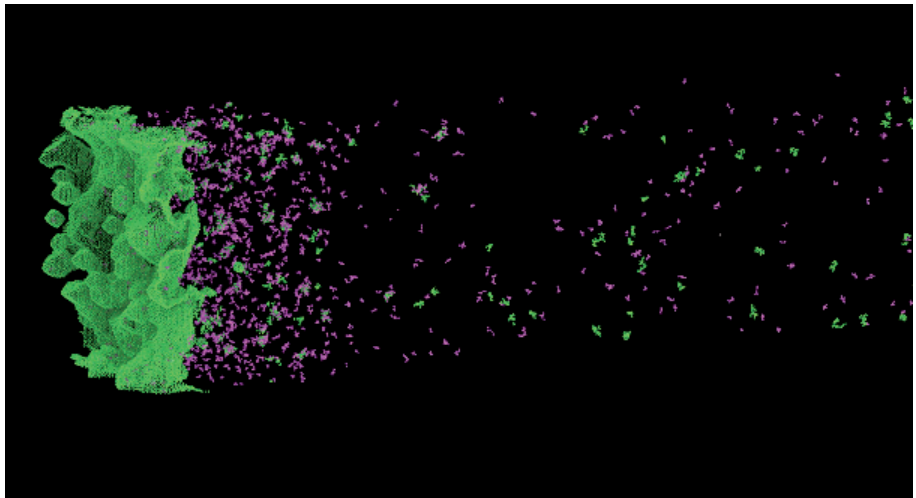
4. External Scientific Member of Leibniz Institute of Polymer Research Dresden.
· **Dr. De-Yi Wang**

5. Best PhD Thesis 2012-2013, Technical University of Madrid
· **Dr. Silvia Hernández**

6. Best PhD Theses 2013/2014, Carlos III University of Madrid
· **Drs. Rocío Muñoz** and **Saeid Loftian**

7. 2014 EPMA Keynote Paper Award, European Powder Metallurgy Association
· **Prof. J. M. Torralba**

awards



institutional activities

6.10. Institutional Activities

- Member of the European Materials Modelling Council (EMMC)
- Member of the Metallurgy Europe Eureka Cluster
- Member of the European Energy Research Alliance EERA AISBL
- Member of the European Composites, Plastics and Polymer Processing Platform (ECP4)
- Coordinator of the Spanish Technological Platform of Advanced Materials and Nanomaterials (MATERPLAT)
- Local Contact Point of the EURAXESS pan-European initiative
- 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).
- Participation in the "*XIV Semana de la ciencia*", promoted by *Fundación Madri+d.*
- Participation in the European Researchers' night Madrid 2014, promoted by *Fundación Madri+d.*

theses

6.11. Theses

6.11.1. PhD Theses

"Formability of ultra-fine grained metallic materials"
Student: Eva Cristina Moreno Valle
Carlos III University of Madrid
Advisor: Dr. I. Sabirov
Date: March 2014

"Virtual development and validation of non-conventional lay-ups"
Student: Olbén Falcó
University of Girona
Co-advisor: Dr. C. S. Lópes
Date: April 2014

"Physical modeling of junction processing in FDSOI devices for 20nm node and below"
Student: Benoît Sklenard
University of Grenoble
Co-advisor: Dr. I. Martín-Bragado
Date: April 2014

"High fidelity simulations of failure in fiber-reinforced composites"
Student: Sergio Sádaba
Technical University of Madrid
Advisors: Dr. C. González and Prof. J. LLorca
Date: June 2014

"Continuum models of the mechanical behavior of rolled and die-cast magnesium alloys"
Student: Ana Fernández
Technical University of Madrid
Advisors: Dr. M. T. Pérez-Prado and Prof. A. Jérusalem
Date: June 2014

"Size effect in LiF plasticity: new insights into the lattice resistance contribution"
Student: Rafael Soler
Carlos III University of Madrid
Advisors: Drs. J. Mikel Molina and J. Segurado
Date: June 2014

"High temperature mechanical behavior of Al/SiC nanoscale multilayers"
Student: Saeid Loftian
Carlos III University of Madrid
Advisors: Dr. J. M. Molina-Aldareguía and Prof. J. LLorca
Date: June 2014

"Mechanical behavior of hybrid 3D woven composites"
Student: Raúl Muñoz
Carlos III University of Madrid
Advisors: Dr. C. González and Prof. J. LLorca
Date: July 2014

"Large scale multiphysics modeling of neurites"
Student: Julian Andres Garcia Grajales
Technical University of Madrid
Advisor: Prof. A. Jérusalem
Date: September 2014

"Processing and properties of high-performance 7075 Al and AZ91 Mg powder metallurgy alloys"
Student: Mohammad Ali Jabbari
Carlos III University of Madrid
Advisor: Prof. J. M. Torralba
Date: November 2014

6.11.2. Master/Bachelor Theses

"Preparation and analysis of the fire behavior of polypropylene based nanocomposites"
Student: Sergio de Juan
Technical University of Madrid
Advisor: Dr. D. Y. Wang
Date: May 2014

"Modeling and Design of Energy Absorption Materials for Impact Loading"
Student: Alejandro García
Carlos III University of Madrid
Advisor: Dr. C. S. Lópes
Date: June 2014

"Synthesis of graphene/inorganic hybrids"
Student: Jorge Elena
Complutense University of Madrid
Advisor: Dr. J. J. Vilatela
Date: June 2014

"Multifunctional nanocomposites based on inorganic/CNT fibre hybrids"
Student: Alfonso Monreal-Bernal
Complutense University of Madrid
Advisor: Dr. J. J. Vilatela
Date: June 2014

"Fire retardant polylactic acid and its properties"
Student: Francisco Reyes
Technical University of Madrid
Advisor: Dr. D. Y. Wang
Date: July 2014

"Numerical simulation of morphing materials: polyamide SDS filled with flexible polyurethane foam"
Student: Leticia Arbelo
Technical University of Madrid
Advisor: Dr. J. Segurado
Date: July 2014

"Generation of polycrystalline microstructures of Ni-based superalloys for finite element method analysis"
Student: Daniel Barba-Cancho
Technical University of Madrid
Advisor: Dr. J. Segurado
Date: July 2014

"Mechanical, thermal and electrical vharacterization of polypropylene nanocomposites"
Student: Luis Carlos Herrera
Technical University of Madrid
Advisor: Dr. R. Guzmán de Villoria
Date: July 2014

"Powder metallurgy invar-carbon nanotubes metal matrix composites"
Student: Miguel Pretus
Carlos III University of Madrid
Advisor: Dr. R. Guzmán de Villoria
Date: July 2014

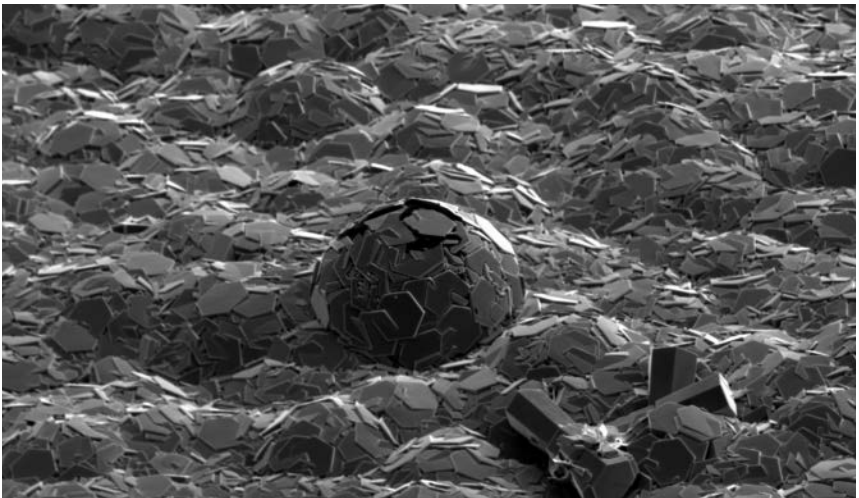
"Dynamic percolation in nanocompositesand its relation to nanocarbon/thermoset electric curing"
Student: Juan Carlos Fernández
Complutense University of Madrid
Advisor: Dr. J. J. Vilatela
Date: September 2014

"Fabrication and characterization of RTM6 nanocomposites"
Student: Ignacio Bolaños
Carlos III University of Madrid
Advosor: Dr. R. Guzmán de Villoria
Date: September 2014

"Análisis paramétrico del método SPH aplicado a la modelización de hielo en impactos sobre estructuras laminadas de material compuesto"
Student: César Chamorro
Carlos III University of Madrid
Advisor: Dr. C. S. Lópes
Date: October 2014

"An experimental and finite element modeling study of the strength of Al/SiC multilayers"
Student: Yang Lingwei
Technical University of Madrid
Advisor: Dr. J. M. Molina-Aldareguia
Date: November 2014.

internship
visiting students



6.12. Internships / Visiting Students

"<100> vs. <111> loops in Iron as modeled with Object Kinetic Monte Carlo"
Student: Maria José Aliaga,
Date: February-March 2014 and October-November 2014
Advisor: Dr. I. Martín Bragado
Visiting student from: University of Alicante, Spain

"Hot workability of NiAl-W in situ composites"
Student: Du Rou
Date: March-August 20
Advisor: Dr. S. Milenkovic
Visiting student from: Academic Internship Programme for Chinese Technical Students offered by the Technical University of Madrid

"Nano inorganic flame retardant /polypropylene composites",
Student: Yvonne Spörer
Date: April-September 2014
Advisor: Dr. D. Y. Wang
Visiting student from: Dresden University of Technology, Germany

"Nano flame retardants in flexible poly(vinyl chloride)"
Student: Cedric Trempont
Dates: May-July 2014
Advisor: Dr. D. Y. Wang
Visiting student from: Ecole Nationale Supérieure de Chimie de Lille, France

"Nanoporous CNT fibre/polymer structures"
Student: Erwin Giraud
Date: May-July 2014
Advisor: Dr. J. J. Vilatela
Visiting student from: Phelma-INP, France

"Synthesis and preparation of flame retardant epoxy resin composites"
Student: Fernandez Florian
Dates: June-August 2014
Advisor: Dr. D. Y. Wang
Visiting studen from: Ecole Nationale Supérieure de Chimie de Lille, France

"Composites"
Student: Marcos Jiménez
Dates: June-July 2014
Advisor: Dr. R. Guzán de Villoria
Visiting student from: Polytechnic University of Valencia, Spain

"Graphene based-composites"
Student: Alejandro Vázquez
Dates: June-August 2014
Advisor: Dr. I. Martín-Bragado
Vistiting student from: Massachusetts Institute of Technology, USA

"X-Ray Computed Tomography characterization of cast Inconel 718"
Student: Bojdan Nedelcu
Dates: July-September 2014
Advisor: Dr. F. Sket
Visiting student from: Carlos III University of Madrid, Spain

"Thermal calibration of a pyrometer and its application for temperature control of casting"
Student: Carolin Hörhager
Dates: July-September 2014
Advisor: Dr. D. Y. Wang
Visiting student from: ERASMUS internship Programme, Germany

"Synthesis of fire retardants for epoxy"
Student: Liang Li
Dates: October-November 2014
Advisor: Dr. D. S. Milenkovic
Visiting student from: Technical University of Madrid, Spain

"Modeling of damage evolution in Fe using MMonCa and Lakimoca"
Student: Monica Chiapetto
Dates: October-November 2014
Advisor: Dr. I. Martín-Bragado
Visiting student from: SCK-CEN, Belgium

6.13. Courses

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

"Simulation of Composite Materials"
Master in Composite Materials
Technical University of Madrid and EADS
Professors: Dr. C. González, Dr. C. S. Lopes, Dr. J. Segurado, S. Sádaba, F. Hergueta

"Structural composite materials"
Master/Doctoral Programme in Materials Engineering
Technical University of Madrid
Professors: Prof. J. LLorca

"Mechanics of composite materials"
Master/Doctoral Programme in Materials Engineering
Technical University of Madrid
Professors: Prof. J. LLorca

"Structural characterization of Materials II: Spectroscopy"
Master/Doctoral Programme in Materials Engineering
Technical University of Madrid
Professors: Dr. F. Sket

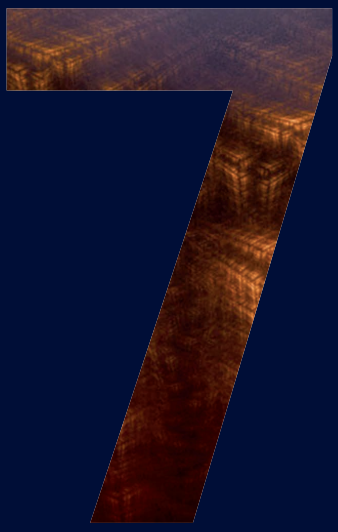
"Simulation in Materials Engineering"
Master/Doctoral Programme in Materials Engineering
Technical University of Madrid
Professors: Dr. C. S. Lópes, Dr. Y. Cui, Dr. I. Martín-Bragado, Prof. J. LLorca

"Impact Behaviour of Materials"
Master/Doctoral Programme in Materials Engineering
Technical University of Madrid
Professors: Dr. C. S. Lópes

"Discretization methods in Engineering"
Master in Seismic Engineering
Technical University of Madrid
Professors: Dr. I. Romero

"Materials and Sustainability"
Degree in Materials Engineering (3rd course)
Technical University of Madrid
Professor: Dr. D. Y. Wang

scientific highlights



annual report 2014

design of

ply material properties

Design of Composite Ply Material Properties

Composite materials reinforced with high performance fibres are preferred candidates in structural applications wherein strength to weight ratio leads the design process. One of the main drawbacks regarding these materials is their complex mechanical behaviour which depends on their orthotropic architecture, properties of their constituents, design variables and manufacturing conditions.

Since the discovery of high-performance glass and carbon fibres, the production process and microstructure of composites have been improved to maximize their mechanical, thermal and chemical properties. However, the morphology of fibres has not evolved from their current circular shape. While it is commonly accepted that the mechanical response of fibre-reinforced polymer plies is a function of the relative fractions of fibres and matrix and on their respective mechanical properties, as well as of the fibre/matrix interface, they ought also to be dependent on the fibre's cross-section shape and microstructural arrangement. This derives from the evidence that fibre shape determines the meandering of the fibre/matrix interface whose behaviour plays a major role on the ply response under transverse and shear loading **[1, 2]**. Furthermore, the cross-section shape of the fibres determines the maximum achievable fibre volume fraction which in turn controls the longitudinal properties.

Non-circular carbon fibres with lobular and ribbon shape have been successfully manufactured in research laboratories, as depicted in Figure 1. While the influence of production parameters (e.g. carbonization temperature) on the mechanical properties of the individual fibres was studied to some extent, their effectiveness in a composite has been scarcely investigated, probably due to the high costs associated with the experimental campaigns.

A coupled experimental-computational multiscale analysis strategy recently developed at IMDEA Materials Institute **[1, 2]** enables accurate virtual testing of composite materials, and prompts the reduction of time- and money-consuming experimental campaigns. Following this approach, ply, laminate and structural properties of composites can be effectively obtained from the behaviour of their micro-constituents and from material design parameters at these three scales, including fibre cross-section shape. The efficiency of such analyses coupled with recent advances in computing power such as parallel GPU acceleration allow the design of enhanced composite microstructures at IMDEA Materials Institute (Figure 2).

References

[1] J. LLorca, C. González, J.M. Molina-Aldareguía and C.S. Lopes, **JOM, 65,** 215, 2013.

[2] J. LLorca, C. González, J. M. Molina-Aldareguía, J. Segurado, R. Seltzer, F. Sket, M. Rodríguez, S. Sádaba, R. Muñoz, L. P. Canal, **Advanced Materials, 23,** 5130 (2011).

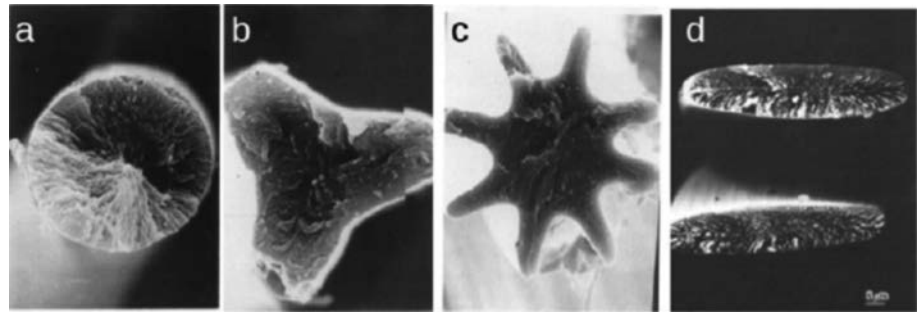


Figure 1. Carbon fibres of different section shapes produced in laboratory

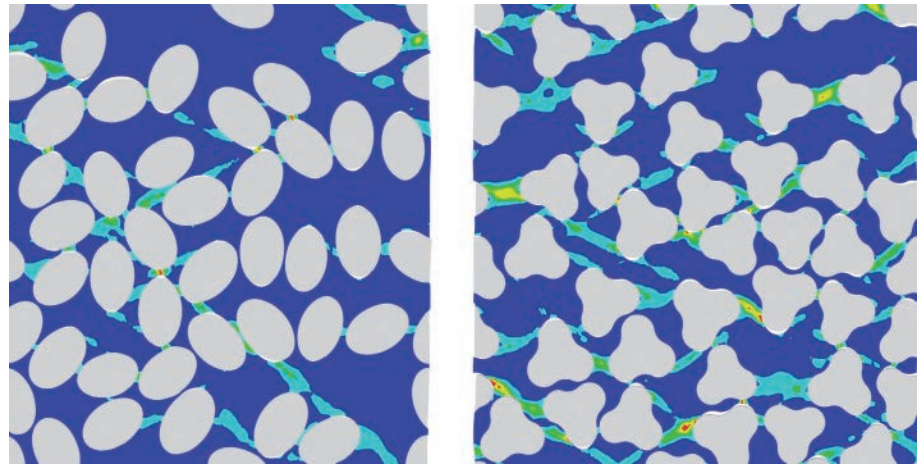


Figure 2. Simulation of the mechanical behaviour of composite plies containing elliptical (left) and lobular (right) fibres under transverse compression.

carbon-based na

multiscale materials design

Carbon-based nano-architectures: Multiscale Materials Design

Carbon nanomaterials, e.g nanotubes or graphene films, present a strong potential for novel engineering applications. Their properties in terms of mechanical strength, electrical and thermal conductivity, transparency, corrosion resistance and surface area, make them ideal candidates to meet the current needs of lighter structural materials for transport or highly efficient energy generation/storage systems. They can be synthesized by chemical vapor deposition (CVD), a very appealing technique in terms of production yield, versatility and scalability.

The Nano-Architectures and Materials Design group at IMDEA Materials Institute has developed an experimental semi-continuous CVD technology especially designed to synthesize graphene, thin carbon films or vertically aligned carbon nanotubes. This facility is able to carry out fast thermal annealing, that permits a high rate of experiments per day.

This unique system provides to IMDEA Materials Institute with a new route to synthesize carbon nanomaterials on low-cost metal foils **[1]**. For example, graphene and thin carbon films synthesized directly on copper foils **[2-3]** can be easily transferred to other substrates by acid etching or direct delamination (Fig. 1), and can be also tested as transparent and flexible electrodes.

In addition, stainless steel foils are used to directly grow vertically aligned carbon nanotubes and carbon films, forming a hybrid nano-material (Fig. 2) **[4]**. This approach reduces significantly the cost, as this process generally needs silicon wafers processed by expensive micro-fabrication techniques. Because of the potential of these nano-structures, applications in the field of energy storage, actuators, composites, etc. are envisioned.

With this unique system, IMDEA Materials Institute is positioned at the forefront of synthesis of nano-architectures, working in one of the most scientifically and technologically exciting fields, as recognized by the European Union and their Flagship program on graphene.

References

[1] R. Guzmán de Villoria, A. J. Hart, and B. L. Wardle, *"Continuous High-Yield Production of Vertically Aligned Carbon Nanotubes on 2D and 3D Substrates,"* **ACS Nano, 5,** 4850–4857, 2011.

[2] S. Bae, H. Kim, Y. Lee, X. Xu, J.-S. Park, Y. Zheng, J. Balakrishnan, T. Lei, H. Ri Kim, Y. I. Song, Y.-J. Kim, K. S. Kim, B. Özyilmaz, J.-H. Ahn, B. H. Hong, and S. Iijima, *"Roll-to-roll production of 30-inch graphene films for transparent electrodes,"* **Nat. Nanotechnol., 5,** 574–578, 2010.

[3] P. Romero and R. Guzman de Villoria, Manuscript in preparation

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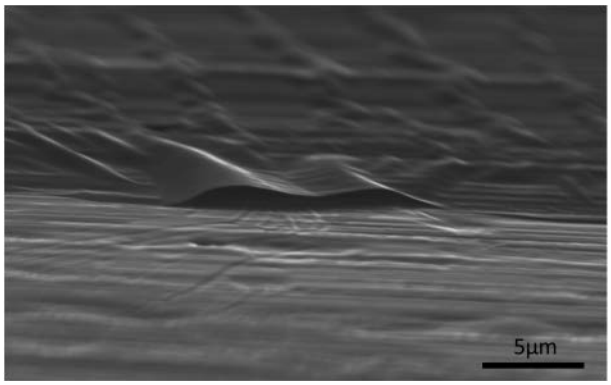

Figure 1. Detail of a thin carbon film synthesized directly on a copper foil.

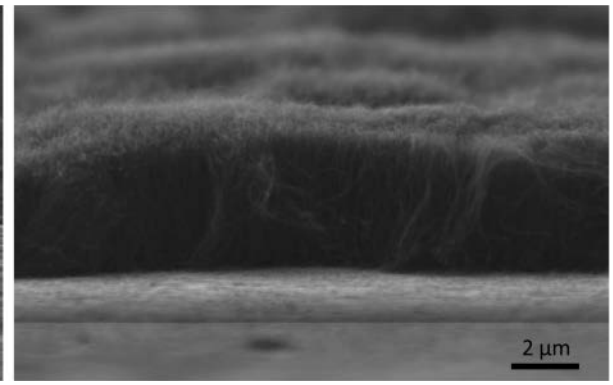

Figure 2. Vertically aligned carbon nanotubes grown directly on a stainless steel foil.

numerical mes

Numerical meshfree methods for solids and fluids under extreme conditions

for solid and fluids under extreme conditions

Traditional simulation techniques for solid mechanics are based on geometrical models obtained from the tessellation of the analysis domain. In particular, Lagrangian finite elements, the most common method for linear and nonlinear solid mechanics, employ simplicial or hexahedral tessellations and are well known to suffer accuracy and stability issues when these meshes are distorted. While re-meshing strategies alleviate such problems, they are costly and introduce undesirable smoothing in the solution.

Given the aforementioned limitations of mesh-based approximations, the Computational Mechanics community has identified the need for developing alternative methods and a large number of mesh-free schemes have been developed in the last two decades. Many advances have been done in this field, but no method is devoid of drawbacks, and a clear winner approximation is yet to emerge.

The Computational Solid Mechanics group at IMDEA Materials Institute has developed a meshfree method that can be employed to approximate the solution of nonlinear problems in solid and fluid mechanics, as well as their interaction. In the solid solver, a Galerkin method with local maximum entropy functions is employed; in the fluid counterpart, a consistent stabilization is used to ensure the robustness of the formulation for incompressible flows. To solve fluid/solid interaction problems, a fully Lagrangian method is implemented also for fluid domains, simplifying the representation of free surfaces, and contact between bodies.

The method developed allows, first, the simulation of nonlinear problems in solid mechanics with very large distortions without the need for remeshing. Four snapshots of a deep-drawing process of a still disk are depicted in figures 1a-1d (one quarter of the punched disk is shown only). The material is elastoplastic with isotropic and kinematic hardening, and the values of the von Mises equivalent stress (expressed in MPa) are shown in the legend. Each dot in this figure is a material point inside the disk and no mesh has been employed. In a second example, four instants of the impact between a water sphere and an elastoplastic plate are shown in Figure 5. As in the solid example, the spheres represent fluid/solid material points.

Even though more advanced features still have to be incorporated into the simulation framework, the developed tools have already become a very competitive alternative to standard simulation techniques, and hold promise to be of great aid in solving problems in manufacturing modeling (extrusion, injection, drawing), impact, fragmentation, wetting, etc.

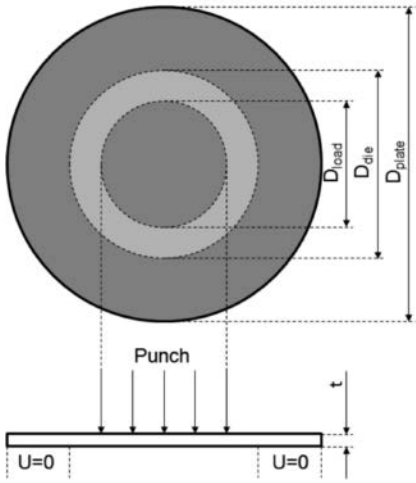

Figure 1. Geometry of the deep drawing example (t=2mm, Dplate = 200 mm, Dload = 75mm)

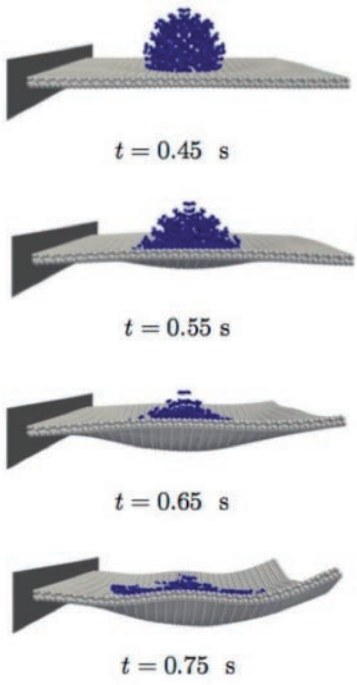

Figure 2. Snapshots of the impact of a water sphere on a deformable plate

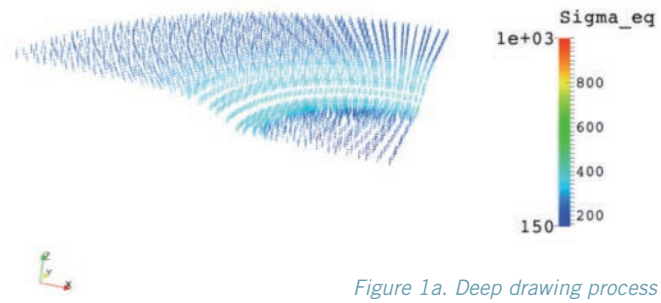

Figure 1a. Deep drawing process

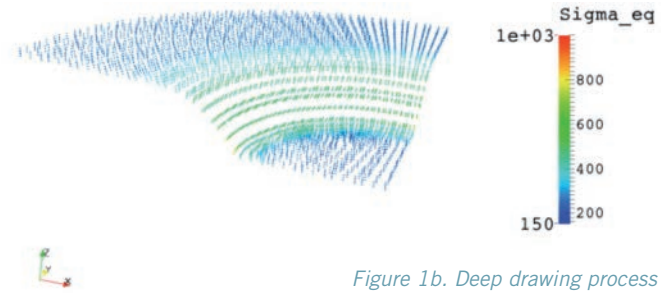

Figure 1b. Deep drawing process

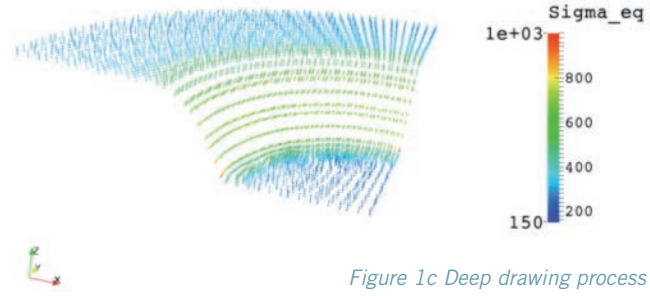

Figure 1c Deep drawing process

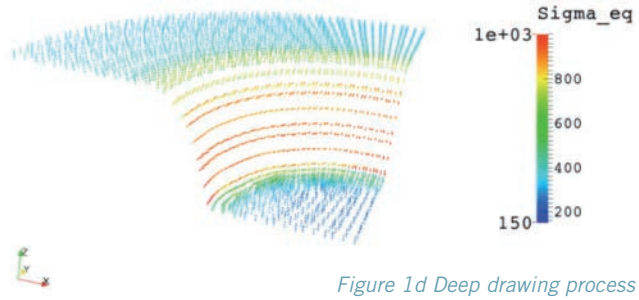

Figure 1d Deep drawing process

high-throughput

High-throughput experimental screening of solidification-microstructure relationships

screening of solidification microstructure relationships

The classical one-at-a-time research methodology to develop new materials limits technological progress, particularly nowadays when engineering design tools have radically reduced the time necessary to optimize new products. New strategies based on combinatorial materials science and high-throughput techniques have been recently introduced to speed up materials innovation. Thin films with discrete composition libraries or continuous composition gradients (spreads) are currently used to study composition–structure–property relationships of complex functional materials in one shot. In contrast, high-throughput methods involving bulk materials are rather scarce and bulk diffusion couples have been just used in metallurgy for the evaluation of diffusion coefficients or the determination of phase diagrams.

A majority of manufacturing processes involve melting and solidification of metallic alloys during fabrication of various components. Nevertheless, the effect of solidification processing variables on the microstructure is still being determined following the one-alloy-at-a-time strategy, and new alloy development remains a very long and costly process. To overcome these limitations, the researchers of IMDEA Materials Institute have introduced a novel high-throughput methodology within the VANCAST project for establishing solidification-microstructure relationships of metallic alloys.

The new strategy is based on melting/solidification experiments with a constant cooling rate and variable temperature gradient in a Gleeble 3800 thermo-mechanical simulator. **[1]** The temperature is measured by four thermocouples welded along the sample to obtain the cooling curves (Fig 1a). These data are used to determine the temperature distribution along the sample (Fig. 1b). Then, the temperature gradient and solidification rate can be precisely determined at any point of the sample. The different solidification rates along the sample leads to different microstructures, and a spread of microstructures corresponding to a range of well-controlled solidification rates is produced in a single melting/solidification experiment. This is shown in Fig. 2, in which different microstructures (characterized by grain size and secondary dendrite arm spacing) were obtained in a single specimen of IN718 Ni-based superalloy corresponding to temperature gradients in the range 1 to 40 K/mm and solidification rates from 0.25 to 10 mm/s **[2]**. This strategy can be employed not only for microstructure prediction in the as-cast complex shape

[1] The VANCAST project was funded by ERA-NET MATERA + within the 7th Framework Program of the European Union. Other project partners included Industria de Turbo Propulsores, Precicast Bilbao, CALCOM-ESI, Swiss University of Applied Sciences and Precicast Novazzano

parts via investment casting, but also for microstructure screening and optimization of all relevant solidification processes, from directional solidification to rapid solidification.

References

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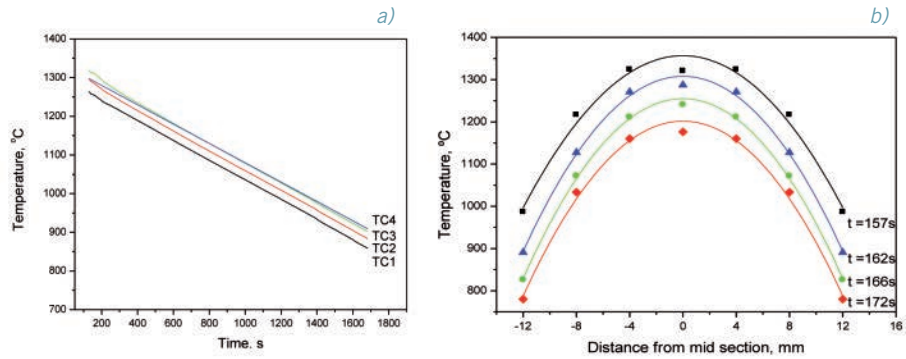
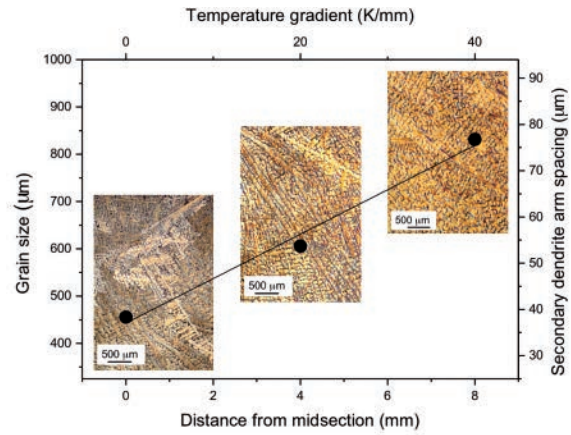


Figure 1. a) Cooling curves recorded by four thermocouples during the melting/solidification experiment; b) Temperature distribution along the sample axes.

Figure 2. Changes in the microstructure (characterized by the grain size and the secondary dendrite arm spacing) with the distance from the midsection of the sample during the high-throughput melting-solidification experiments in a Gleeble 3800 thermo-mechanical simulator.



a polycrysta

A polycrystalline model for a Ni-based superalloy based on micro-pillar compression tests

for a Ni-based superalloy based on micro-pillar compression tests

Computational homogenization is an ideal tool to predict the mechanical properties of polycrystalline alloys taking into account the microstructure. This methodology is based on the numerical simulation (normally by means of the finite element method) of the mechanical behavior of a Representative Volume Element (RVE) of the microstructure that accurately reproduces the grain size, shape and orientation distributions **[1]**. The behavior of the grains is modeled using a Crystal Plasticity (CP) model that accounts for the anisotropic elastoplastic response due to lattice deformation and dislocation slip and/or twinning **[2]**.

IMDEA Materials Institute, in collaboration with ITP, has developed a novel multiscale modeling strategy based on computational homogenization to obtain the mechanical properties of cast and wrought Ni-based superalloys used in aeroengine gas turbines. The roadmap of this multiscale strategy is depicted in Figure 1 and begins by an accurate description of the polycrystalline microstructure (in terms of grain size, shape and orientation) by means of optical microscopy, electron-backscatter diffraction as well as X-ray diffraction. Afterwards, the mechanical properties of single crystals are obtained from compression tests in a nanoindenter of micron-sized pillars milled from the grains in the polycrystal by means of focus ion milling. The micropillar tests are carried out in a range of temperatures and strain rates in different orientations (to promote single and multiple slip) and are used as input to obtain the parameters of the CP model that can reproduce the single crystal behavior. This model is used as the constitutive equation of the individual grains in the numerical simulation of an RVE of the microstructure, which provides the mechanical response of the polycrystalline Ni-based superalloy under the corresponding load history (uniaxial and multiaxial loading, static and cyclic loading, creep, etc.)

The result of this methodology to predict the stress-strain curve in compression of a wrought Inconel 718 superalloy is shown in Figure 2. This alloy is widely used in structural components for aeroengines due to its excellent corrosion resistance and mechanical properties up to 650ºC. The RVE of the microstructure (Fig. 2a) was built from the experimental log-normal distribution of grain sizes using a Voronoi tessellation. The grain orientation was random and the grain size equiaxed, according to the experimental data. The RVE of the microstructure included 210 grains and each grain was discretized with approximately 600 finite elements to obtain an accurate description of the strain and stress fields within each grain. The mechanical response of the polycrystal under uniaxial loading at room temperature obtained by the multiscale approach is compared in Fig. 2b with the experimental results. The model predictions were very close to the experimental data (differences were under 5%) and this agreement is remarkable taking into account that all the models parameters (that define the microstructure and the mechanical behavior

of single crystals) were obtained from independent experiments. This example highlights the potential of the novel multiscale framework to carry out virtual tests of polycrystalline materials that include the influence of the microstructure on the mechanical response.

This investigation has been supported by the project MICROMECH ("Microstructure Based Material Mechanical Models for Superalloys"), funded by the 7th Framework Program of the European Union within the Clean-Sky JU call.

References

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[2] V. Herrera-Solaz, J. LLorca, E. Dogan, I. Karaman, J. Segurado. *An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests: application to AZ31 Mg alloy,* **International Journal of Plasticity, 57,** 1–15, 2014.

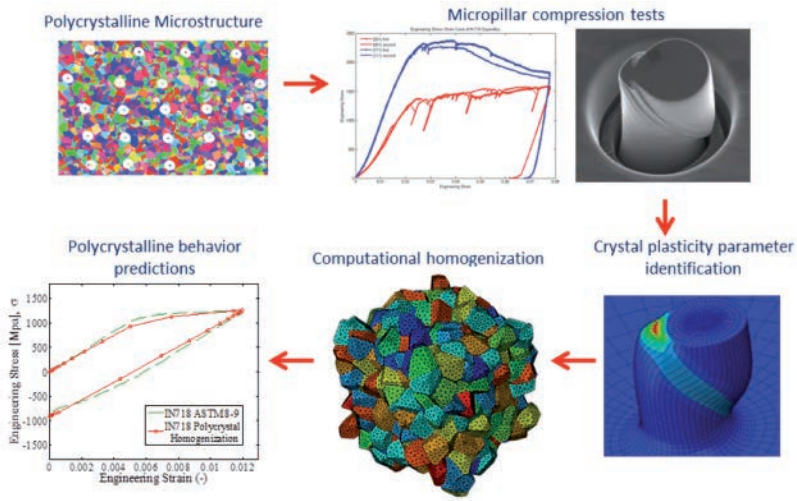

Figure 1. Multiscale modeling strategy to obtain the mechanical behavior of polycrystalline Ni-based superalloys.

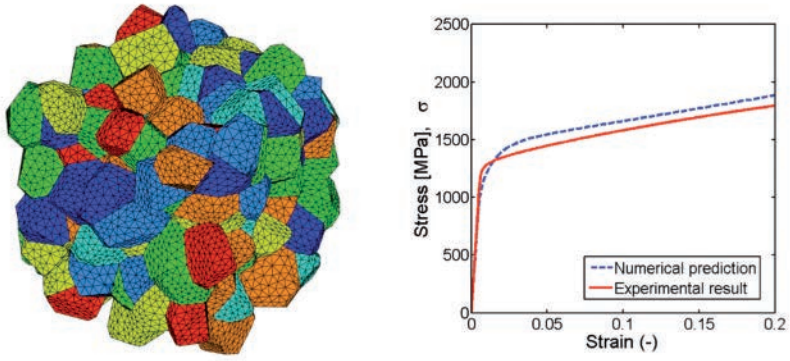

Figure 2. (a) RVE of the microstructure of a wrought Inconel 718 alloy. Individual grains with different orientations are shown with different colors. (b) Experimental results and numerical predictions of the mechanical behavior of polycrystalline Inconel 718 under uniaxial compression at ambient temperature.

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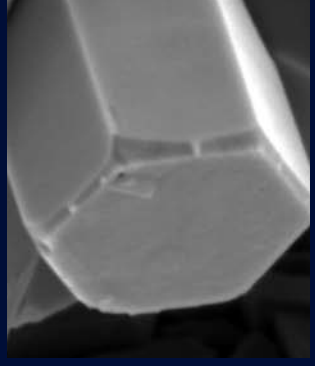

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