foreword

Javier LLorca
Director, IMDEA Materials Institute
March 2015

annual report

2015
Institutions are designed, created and run by people but the institution remains while people come and go as time passes by. After eight years as the chairman of the Board of Trustees, Dr. Pedro Muñoz-Esquer has stepped down although he will continue with us as a member of the Scientific Council. The IMDEA Materials Institute is indebted to the continuous guidance and encouragement of Dr. Muñoz-Esquer -an engineer and an academic who pioneered the use of composite materials in civil aircraft during his tenure at Airbus- to combine excellence in research together with technology transfer to industry. The Board of Trustees has appointed Prof. Juan Manuel Rojo, emeritus professor of the Complutense University of Madrid, as the new chairman of the board. Prof. Rojo is a member of the Spanish Royal Academy of Sciences and has an international reputation in surface science. In addition, he was the Spanish Secretary of State for Universities and Research (1985-1992) and a member of the IMDEA Materials Institute’s Board of Trustees (2007-2013) on behalf of the Complutense University of Madrid.

In addition, Prof. Ignacio Romero, who leads the research group on Computational Solid Mechanics, has been designated as Deputy Director of the Institute. He takes over the position of Prof. José Manuel Torralba, who has been appointed General Director for Universities and Research by the Regional Government of Madrid. Fortunately, we are not losing José Manuel, as he will continue with us as a member of the Board of Trustees on behalf of the regional government.

As a result of the Institute’s continuous growth, which has reached 100 people, the Scientific Council recommended the re-organization of the research programmes and the creation of a new programme on the Multiscale Characterization of Materials and Processes. The new programme is focussed on 3D characterization of materials, including microstructural, chemical and crystallographic analysis across multiple length scales (from nm to mm) as well as on in situ characterisation across multiple scales (4D characterisation). The activities of the programme are endowed with state-of-the-art facilities that include transmission and scanning electron microscopy, X-ray microtomography, ion beam micromachining and patterning as well as in situ stages for studying the kinetics of processes (mechanical, thermal, chemical, etc.) from the nm to mm scale up to 700 °C. In addition, the research programme on Integrated Computational Materials Engineering was reinforced with the opening of a new research group on Computational and Data-Driven Materials Discovery, which adds a different perspective to the use of computational tools to discover and design new materials for engineering applications.

The outcome of the research activities performed during 2015 is summarized in the following pages. They show that the IMDEA Materials Institute continues its path towards becoming an international reference in the discovery and development of new materials, mainly for transport, energy, information technology and manufacturing, as well as in the exploration of emerging materials and processes for sustainable development.
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1.1. About the IMDEA Materials Institute

The IMDEA Materials Institute (Madrid Institute for Advanced Studies of Materials) is a non-profit independent research organisation 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 work in Madrid in an international and interdisciplinary environment.

Research approach

The IMDEA Materials Institute combines oriented fundamental research with applied research addressing the scientific and technological challenges that drive innovation in Materials Science and Engineering. The Institute’s research groups, the “building blocks” of the centre, are led by top scientists working at the forefront of knowledge in emerging fields related to industrial needs.

Another aspect of the Institute’s research activity is the interdisciplinarity that is introduced by the close collaboration among different research groups at the intersection of complementary research fields to maximise scientific impact and technological leadership. This interdisciplinary approach is internally promoted through the channelling of our investigations by means of Research Programmes with clear scientific and technological goals, which are achieved as a result of the synergistic contributions of the different groups. Moreover, strategic R&D collaborations are established with research groups and industrial partners outside of the Institute to incorporate the diverse expertise necessary to achieve the goals.

The combination of excellence in research with the ability to address technological challenges allows the IMDEA Materials Institute to collaborate efficiently with companies to create value in their products and processes through novel knowledge that will be transformed into technological innovations.

The Institute’s research team approaches its R&D activities from two different perspectives that are always founded on excellence in research. The first one is a bottom-up
approach which goes from the fundamentals to the applications where key scientific knowledge (i.e. breakthroughs) is generated to develop or improve materials and/or processes leading to industrial innovations. The second approach is a top-down strategy that begins with a technological challenge for an application identified by industry. The research is then focused on the fundamentals that allow the real understanding of the problem and enabling a solution to be designed, leading to a strategy that goes from the applications to the fundamentals.

Figure 1. Bottom-up (fundamentals to applications) and top-down (applications to fundamentals) research approaches of IMDEA Materials Institute.
1.2. Appointments to the Board of Trustees and Scientific Council

Prof. Juan Manuel Rojo, Emeritus Professor of the Complutense University of Madrid has replaced Dr. Pedro Muñoz-Esquer as scientific trustee and Chairman of the Foundation.

Prof. Rafael van Grieken Salvador, Counsellor of Education, Youth and Sports replaced Mrs. Lucía Figar de Lacalle as Vice-Chairman of the Foundation.

Prof. José Manuel Torralba, General Director of Universities and Research of the Madrid Regional government replaced Mrs. Lorena Heras Sedano as one of the permanent trustees from the Regional Government of Madrid.

Prof. Rafael A. García Muñoz, Deputy Director of Research of the Madrid Regional Government replaced Prof. Juan Angel Botas Echevarría as one of the permanent trustees from the Regional Government of Madrid.

Prof. Francisco Javier Prieto, Vice-President for Research at Carlos III University, replaced Prof. Carlos Balaguer, as trustee from universities and public research institutions.

Mr. Javier Villacampa, Corporate Innovation Director, has replaced Mr. Fernando Rey as trustee in representation of Grupo Antolín S. A.

In addition, Prof. Mauricio Terrones, Professor of Materials Science and Engineering, The Pennsylvania State University, has been appointed to the Scientific Council.

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

[Image of the organizational chart]

Figure 2. Organizational chart of IMDEA Materials Institute
1.4. Governing Bodies

Members of the Board of Trustees

CHAIRMAN OF THE FOUNDATION

Prof. Juan Manuel Rojo
Emmeritus Professor
Complutense University of Madrid, Spain

VICE-CHAIRMAN OF THE FOUNDATION

Excmo. Sr. D. Rafael van Grieken Salvador
Counsellor of Education, Youth and Sports
Madrid Regional Government

PERMANENT TRUSTEES (REGIONAL GOVERNMENT)

Excmo. Sr. D. Rafael van Grieken Salvador
Counsellor of Education, Youth and Sports
Madrid Regional Government

Ilmo. Sr. D. José Manuel Torralba Castelló
General Director for Universities and Research
Madrid Regional Government

Dr. Rafael A. García Muñoz
Deputy General Director for Research
Madrid Regional Government

Mr. José de la Sota Rius
Coordination of the Area of Investigation, Development and Innovation
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. Francisco Javier Prieto
Vice-President for Research
Carlos III University of Madrid, Spain

SCIENTIFIC TRUSTEES:

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

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

Prof. Trevor William Clyne
Professor
Cambridge University, UK

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

Prof. Juan Manuel Rojo
Emmeritus Professor
Complutense University of Madrid, Spain

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. Javier Villacampa,
Corporate Innovation Director
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 Alcobendas,
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. Dr. Dierk Raabe  
Director, Max-Planck Institute for Iron Research Professor  
RWTH Aachen University, Germany

Prof. Gary Savage  
Independent consultant

Prof. Mauricio Terrones  
Professor, The Pennsylvania State University, USA

Prof. John R. Willis  
Professor  
Cambridge University, UK
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2.1. Research Programmes

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

- Nanomaterials for Multifunctional Applications
- The Next Generation of Composite Materials
- Alloy Design, Processing and Development
- Integrated Computational Materials Engineering
- Multiscale Characterisation of Materials and Processes

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, characterisation 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 programmes.

Driven by the talent of the researchers, research programmes combine cutting-edge fundamental oriented research in topics at the frontiers of knowledge with applied research encompassing the midterm interest of our industrial partners to provide long-term technological leadership.

Figure 3. Research programmes and strategic partners of IMDEA Materials Institute
Nanomaterials for Multifunctional Applications

- Synthesis, emerging technologies and integration of carbon-based nanomaterials (graphene, nanotubes, nanofibers and hybrids):
  - Sensors: chemical, piezoresistive, piezoelectric.
  - Size effects in the mechanical behaviour of multifunctional materials: strength of graphene, nanotubes, nanofibers, fibers and their interfaces.

- Synthesis and properties of polymer-based multifunctional nanocomposites:
  - New polymers through nano- and molecular-design: new generation of high performance fire safety polymer-based materials with improved properties (mechanical, thermal, resistance to chemicals and ultraviolet radiation).
  - Multifunctional nanocarriers for novel fire retardant technologies: i) nanotechnology to improve fire resistance of polymers (polymer nanocomposites, nanocoatings, gas and condensed phase mechanisms of fire retardancy); ii) reactive processing (relationship between flame retardants, nanomaterials and polymers during polymer processing).

- Design of environmental-friendly materials:
  - Innovative plastic formulations using new generation of less toxic and/or bio-based additives and polymers.

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

- Computational and Data-Driven Materials Discovery:
  - Discovery of porous materials for various industrial applications such as catalysis and separations.
  - Design of ionic liquids with precisely tuned properties for a given application.
  - Identification of structure-property relationships and other design rules through high-throughput simulation techniques.
  - Data-mining of scientific literature and material databases to find new lead materials.
Research groups involved:

- Multifunctional Nanocomposites (Dr. J. J. Vilatela, Programme Leader)
- Nano-architectures and Materials Design (Dr. R. Guzmán de Villoria)
- High Performance Polymer Nanocomposites (Dr. D. Y. Wang)
- Computational and Data-Driven Materials Discovery (Dr. M. Haranczyk)

The Next Generation of Composite Materials

- **Processing of high performance composites:**

- **Recycling and repair of structural composites:**

- **New frontiers of structural performance:**

- **Composites with multifunctional capabilities:**

- **Micromechanics of composites:**
  - In situ measurement of matrix, fiber and interface properties. Micromechanics-based failure criteria. Computational design of composites with optimum 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. Behaviour of 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. Lópes)
- Multifunctional Nanocomposites (Dr. J. J. Vilatela)
- Nano-architectures and Materials Design (Dr. R. Guzmán de Villoria)
- High Performance Polymer Nanocomposites (Dr. D.-Y. Wang)
- Nanomechanics (Dr. J. M. Molina-Aldareguía)
- X-ray Characterisation of Materials (Dr. F. Sket)

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. 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 the fabrication of quenched and partitioned steels with superior mechanical properties. Analysis of processing-microstructure-properties relationship on macro- and microscales with emphasis on their strength, ductility, 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. Manufacturing 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 modelling (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 behaviour of single crystals and polycrystals. Implementation of the constitutive models in finite element codes to simulate the mechanical behaviour.

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

**Research groups involved:**

- Physical Metallurgy (Dr. T. Pérez-Prado, Programme leader)
- Solid State Processing (Dr. A. García-Junceda)
- Solidification Processing and Engineering (S. Milenkovic)
- Physical Simulation (Dr. I. Sabirov)
- Multiscale Materials Modelling (Dr. J. Segurado)
- Computational Alloy Design (Dr. Y. Cui)
- X-ray characterisation of materials (Dr. F. Sket)
- Mechanics of Materials (Prof. J. LLorca)
Integrated Computational Materials Engineering

• 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.)
  - Materials for energy generation and storage.

• Materials modelling at different length and time scales:
  - First principles 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 and mechanics
  - Material informatics for analysis of large material datasets
  - Data-driven materials design

• Multiscale materials modelling:
  - Bottom-up approaches (scale bridging)
  - Development of modular multi-scale tools
  - High throughput screening integration
  - Concurrent models
  - Homogenization theory
  - Modelling and simulation of multiscale transport phenomena (application to advanced materials for batteries)

Research groups involved:

• Design and Simulation of Composite Structures (Dr. C. Lopes, Programme Leader)
• Mechanics of Materials (Prof. J. LLorca)
• Multiscale Materials Modelling (Dr. J. Segurado)
• Computational Alloy Design (Dr. Y. Cui)
• Computational Solid Mechanics (Prof. I. Romero)
• Computational and Data-Driven Materials Discovery (Dr. Maciej Haranczyk)
• Atomistic Materials Modelling (Dr. Ignacio Martín-Bragado)
Multiscale Characterisation of Materials and Processes

- **3D Characterisation of materials**, including microstructural, chemical and crystallographic information across several scales and using different techniques:
  - X-Ray Tomography (XCT) and Diffraction (XRD)
  - FIB-FEGSEM, including 3D-SEM, 3D-EDS and 3D-EBSD
  - TEM, including 3D-STEM and 3D-EDS
  - Multiscale correlative tomography studies, i.e. tomography across multiple scales & combining insights from different techniques

- **In-situ characterisation of processes across multiple scales (4D characterisation)**:
  - *Mechanical testing across several length scales*: tension, compression, fatigue, creep, ... of advanced metallic alloys and composites in the SEM and XCT. Properties and deformation mechanisms of small volumes by nanomechanical testing in SEM & TEM: properties of metallic phases, interfaces, nanoparticles, carbon based nanomaterials (carbon nanotubes, graphene, ...).
  - *Elevated temperature nanomechanical testing*
  - *4D characterisation of forming processes by XCT*: Infiltration and resin flow in composites. Solidification of metallic alloys

- **Cross-correlation between experiments and multiscale simulations** (molecular dynamics, dislocation dynamics, crystal plasticity, finite elements, ...)

**Research groups involved:**

- Micro- and Nanomechanics (Dr. J. M. Molina-Aldareguía, Programme Leader)
- X-Ray Characterisation of Materials (Dr. F. Sket)
- Multifunctional Nanocomposites (Dr. J. J. Vilatela)
- Structural Composites (Dr. C. González)
- Physical Metallurgy (Dr. T. Pérez-Prado)
- Multiscale Materials Modelling (Dr. J. Segurado)
- Mechanics of Materials (Prof. J. LLorca)
people

3.1. Senior Researchers [22]
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IMDEA Materials Institute is committed to attract talented researchers from all over the world to Madrid to work in an international and interdisciplinary environment. The Institute currently counts with 16 staff researchers, 5 visiting researchers, 24 post-doctoral researchers and 54 PhD students from 16 different nationalities plus approximately 20 master students. It should be noted that 41% of the researchers are foreign nationals while 57% of the PhD were granted by foreign Universities. This international team with multidisciplinary expertise is contributing to establish IMDEA Materials Institute as an international reference in Materials Science and Engineering. The researchers are supported by six Laboratory Technicians and the Management and Administrative staff, including an international Project Office.

IMDEA Materials Institute endorsed in 2007 the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers that set out the rules and obligations of researchers, their employers and funders, as well as transparent and fair recruitment procedures. The Institute received the ‘Human Resources Excellence in Research’ award from the European Commission on 2015.

**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**
Development of novel multiscale simulation strategies to carry out virtual design, virtual processing and virtual testing of engineering materials for structural applications; experimental characterisation techniques to measure the mechanical properties of materials under extreme conditions at microscopic and macroscopic levels, and analysis of the relationship between microstructure and mechanical properties in advanced structural materials.

**Prof. Ignacio Romero**
Deputy Director, Computational Solid Mechanics
Ph.D. in Civil Engineering, from University of California Berkeley, USA
Professor of Mechanical Engineering, Technical University of Madrid

**Research Interests**
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. Maciej Haranczyk  
(New incorporation)
Senior Researcher, Computational and Data-Driven Materials Discovery

Ph.D. in Chemistry from University of Gdansk, Poland

Research Interests
Computational and data-driven materials discovery and design. His work effectively combines novel materials informatics approaches with traditional computational material science techniques such electronic structure calculations and/or molecular simulations. Moreover, his work often requires leveraging on the recent developments in applied mathematics and computer science.

Dr. Claudio Saul Lopes  
Senior 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. 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. 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 and transmission electron microscopes.

Dr. Srdjan Milenkovic
Senior 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. 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.

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. 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. Juan José Vilatela
Senior 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.

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.
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. Federico Sket
(New incorporation)
Researcher, X-ray Characterisation of Materials
Ph.D. in Materials Engineering from Max-Planck Institute for Iron Research. Germany

Research Interests
Microstructural evolution of metal alloys and fiber-reinforced composites for engineering applications using advanced laboratory and synchrotron X-ray tomography as well as X-ray diffraction. Processing of composite materials and relationship between processing conditions and microstructural evolution. Mechanical deformation of materials and evolution of mechanical and microstructural properties. Development of in-situ devices (based on in-situ X-ray microtomography and X-ray diffraction) for testing mechanical properties and processing using X-rays. Incorporation of experimental results to the development of physically-based models for optimization of material processing and properties.
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 characterisation of biocompatible and biodegradable polymer composites.

Dr. Qinghong Kong
Visiting Scientist, Eco-friendly Fire Retardant Materials
Ph.D. in Safety Science and Engineering from University of Science and Technology of China, China
Associate Professor of Environmental and Safety Engineering, Jiangsu University, China
Research Interests
Synthesis, characterisation and properties of inorganic nanomaterials. Preparation of polymer/inorganic nanocomposites, 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 of Materials Science and Engineering, Guilin University of Electronic Technology, 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. Rigoberto Burgueño
Visiting Scientist, Structural Engineering
Ph.D. in Engineering Sciences from the University of California, San Diego, USA
Professor of Structural Engineering, Michigan State University, USA.
Research Interests
Multiscale assessment and design of tailored materials, devices and structures. In particular: development of mechanical metamaterials using elastic instabilities; hybrid nano- and micro-structured material systems; multiscale modelling and simulation; design optimization of materials and structures; solid and structural mechanics; hybrid structural systems; experimental characterisation of materials and structures; soft-computing methods for structural integrity assessment; inelastic response of concrete structures; and earthquake engineering.

Dr. Arnaud Weck
Visiting Scientist, Fracture at the Microscale
Ph.D. in Materials Science and Engineering from McMaster University, Ontario, Canada
Associate Professor of Mechanical Engineering, University of Ottawa, Canada.
Research Interests
Relationship between microstructure and mechanical properties of materials with particular emphasis on the mechanisms leading to material fracture. The strength and fracture response of materials is investigated using ultrafast lasers to induce artificial defects in materials. The growth of these defects is then studied in-situ under optical and electron microscopes or using high resolution x-ray tomography. Advanced finite element simulations combined with crystal plasticity and nonlocal damage models are used to predict the deformation and fracture of complex materials.
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, characterisation 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 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. Juan Ignacio Beltrán
Postdoctoral Research Associate
Ph.D. in Physics from Autonomous University of Madrid, Spain
Research Interests
Ab-initio based modelling of interfaces to rationalise the relation between atomistic and electronic structure for designing materials with application in electronics, multiferroics and/or magnetism.

Dr. Laura Cabana
Postdoctoral Research Associate
Ph.D. in Materials Science from Autonomous University of Barcelona, Spain
Research Interests
Growth of nanostructures with multifunctional properties. Investigation of strategies for the scaling up production of nanomaterials at the macroscale. Optimization of the production method to obtain a highly pure material. Study of the change in the nanostructure properties after a purification treatment has been conducted. Investigation of the effects of the purification when forming nanocomposite materials for different applications.
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 characterisation of multilayer materials with high damage tolerance based on high-strength aluminium alloys for aerospace applications.

Dr. Hyung-Jun Chang
Postdoctoral Research Associate
Ph.D. in Materials Engineering from Grenoble INP, France and Seoul National University, South Korea
Research Interests
Multiscale materials modelling (molecular dynamics, dislocation dynamics, crystal plasticity and finite elements) and fundamental theories (crystal plasticity, dislocation dynamics, size effects and texture) with applications to macroscale (fracture, hydroforming, equal channel angular pressing, drawing and friction stir welding) and nanoscale (void growth and nanoindentation).

Dr. 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 Dye-Sensitized Solar Cells (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), modelling of fretting and wear, structural integrity.

Dr. Olben Falcó
Postdoctoral Research Associate
Ph.D. in Mechanical Engineering from University of Girona. Spain
Research Interests

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 characterisation, 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. Diego Garijo
Postdoctoral Research Associate
Ph.D. in Aerospace Engineering from Technical University of Madrid. Spain
Research Interests
Computational mechanics (finite element, spectral and meshless methods), composite materials, fracture mechanics, structural health monitoring and optimization.

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. Sandip Haldar
Postdoctoral Research Associate
Ph.D. in Mechanics and Materials at the University of Maryland, College Park. USA
Research Interests

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 nano-composites, 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. 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. David Portillo
Visiting Postdoctoral Research Associate
Ph.D. in Nuclear Fusion from Polytechnic University of Madrid, Spain
Research Interests

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. 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 Engineering from Katholieke Universiteit 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
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Research: Co-based superalloys for high temperature applications

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Research: Solidification and casting

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Research: Vacuum-assisted infiltration and microfluid flow

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Research: Impact in composite materials

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Research: Micromechanics of Ni superalloys

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Research: High-performance polymer nanocomposites

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Research: Development of coating on nanostructured Ti for biomedical application  

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Research: Nanohybrids for photocatalysis  

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Research: Fire retardant polymeric materials  

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Research: Nanostructured supercapacitors
Xiaomin Zhao
MEng: Shanghai Jiao Tong University, China
Research: Polymer nanocomposites

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Research: Voids in out-of-autoclave prepregs

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Research: Advanced NiAl-based eutectic alloys

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Research: Processing of composites by infiltration

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Research: Computational Thermodynamics of Magnesium Alloys

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Research: High throughput diffusion and phase transformation

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Research: Computational alloy design

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Research: Ecofriendly polymer nanocomposites

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Elena Bueno
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Technology Manager
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R&D Project Manager

Raquel García
R&D Project Manager

Borja Casilda
R&D Project Management Assistant
4.1. New research infrastructure [42]
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4.1. New research infrastructure

The following facilities became operational along year 2015. They are further described in the following sections:

- **Arc Melting and Casting Furnace** (Arc 200, Arcast Inc.)
- **X-ray Diffractometer** (Empyrean, PANalytical)
- **Micro Compounder** (MC 15, Xplore)
- **Gel Permeation Chromatographer** (2414, Waters)
- **Field-Emission Transmission Electron Microscope** (Talos F200X, FEI)
- **RAMAN micro-Spectroscopy system** (Renishaw, PLC)
- **In-situ Nanoindenter to carry out elevated temperature mechanical testing inside a SEM** (PI87, Hysitron)

4.2. Processing

- **Arc Melting and Casting Furnace (2015 new equipment)** (Arc 200, Arcast Inc.) for melting, alloying, casting, rapid solidification and atomization of reactive and high melting point elements and alloys up to 3500°C using a clean ceramic free cold crucible process. The furnace offers many options including: tilt casting, centrifugal casting, suction casting, zone melting and gas atomization under inert atmosphere or high vacuum.

- **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.

- **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.
• **Planetary Mills** (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.

• **Micro compounder (2015 new equipment)** (MC 15, Xplore) for compounding thermoplastic based materials or polymeric materials with minute amounts of costly synthesized materials and additives. It has a base capacity of 15 ml. and a maximum torque value is 9000 Nm. Equipped with co-rotating and counter-rotating screws.

• **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.

• **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.

• **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).

• **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 – 100°C.

• **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.

- **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 400°C). Both thermoset and thermoplastic matrix composites can be processed.

### 4.3. Microstructural Characterisation

- **Field-Emission Transmission Electron Microscope (2015 new equipment)** (Talos F200X, FEI) combines outstanding high-resolution S/TEM and TEM imaging with an energy dispersive X-ray spectroscopy integrated system fully compatible with high-resolution 3D tomography. It is also equipped with a PicoIndenter platform to perform *in situ* tests.

This equipment is available to external users through the webpages of the National Center of Microscopy ([www.cnme.es](http://www.cnme.es)) and IMDEA Materials Institute ([www.materials.imdea.org](http://www.materials.imdea.org)).
• **Dual-Beam Focus Ion Beam-Field Emission Scanning Electron 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.

• **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.

• **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 250°C.

• **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.

• **RAMAN micro-Spectroscopy system (2015 new equipment)** (Renishaw, PLC) for obtaining the vibrational spectra of the molecular bonds. It is fully equipped with a Leica DM2700 microscope with 5x, 20x, 50x, 100x objectives, a 532nm Nd:YAG laser (50 mW at 532 nm) and a diffraction grating of 1800 l/mm. It is also equipped with a scanning stage for advanced mapping with 112x76x20 mm range and 100 nm resolution.

• **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).

• **X-ray Diffractometer (2015 new equipment)** (Empyrean, PANalytical) for phase analysis, texture, and residual stress determination, as well as reflectometry. It is equipped with a state-of-the-art X-ray platform for the analysis of powders, thin films, nanomaterials and solid samples. The device is furnished with exchangeable tubes of Cu and Cr radiation, with three sample stages (standard, reflection-transmission spinner and Chi-Phi-x-y-z), an automated sample changer, and a linear detector (PIXcel 1D).
• **Gel Permeation Chromatographer (2015 new equipment)** (2414, Waters) that includes a Waters 2414 refractive index detector, a Waters 2489 UV/Visible detector, a Waters 1500 column heater, and a series of Waters polystyrene GPC columns. It is used to determine molecular weight and molecular weight distribution of soluble polymers or oligomers. It can detect effective molecular range of 100-600,000 Da, with THF or DMF as the mobile phase and an upper limiting temperature of 60 °C.

• **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).

• **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.

• **4.4. Mechanical Characterisation**

• **Dual Column Universal Testing System** (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.

• **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.

• **Fatigue Testing System** (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 -150°C and 350°C.

• **Drop Weight Impact Test System** (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 (FAVIMAT+) 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.

• Nanoindentation System (TI950, Hysitron) to perform instrumented nanoindentation, as well as other nanomechanical testing studies, such as micropillar compression in a range of materials, including test at temperatures up to 500°C. 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.

• In-situ Nanoindenter (2015 new equipment) (PI87, Hysitron) to carry out elevated temperature mechanical testing inside a scanning electron microscope for the in-situ observation of the deformation mechanisms. The stage allows the simultaneous acquisition of the load-displacement record and of the SEM images during mechanical testing (nanoindentation, micro-compression, micro-bending, micro-tension) of micrometer and sub-micrometer size volumes, including elevated temperature testing.

• 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.

• Micromechanical Testing, focused ion-beam, scanning ultrasonic, or atomic force microscopy. Two stages for tension/ Stages (Kammrath and Weiss) to observe the specimen surface upon loading under light, scanning electron 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 700°C.

• Nanoindenter 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.
• **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.

• **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 Characterisation**

• **Micro-scale Combustion Calorimeter** (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, CO₂ and CO yields, effective heat of combustion, and specific extinction areas are directly measured according to ASTM/ISO standards.
• **UL94 Horizontal/Vertical Flame Chamber** (Fire Testing Technology), a widely used flame testing methodology, for selecting materials to be used as enclosures for electronic equipment and other consumer applications. Tests performed include horizontal burning test (UL94 HB), vertical burning test (UL94 V-0, V-1, or V-2), vertical burning test (5VA or 5VB), thin material vertical burning test (VTM-0, VTM-1 or VTM-2), and horizontal burning foamed material test (HF-1, HF-2 or HBF).

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

• **Differential Scanning Calorimeter** (Q200, TA Instruments) to analyse thermal properties/phase transitions of different materials up to 725°C. 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 –40°C to 400°C and high cooling rates of ~50°C/min.

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

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

**4.6. Simulation**

• High Performance Computer cluster with 660 Intel Xeon CPU cores and NVIDIA GPU acceleration leading to a computer power of 90 Tflops

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

• Commercial and open sources software tools for modelling and simulation in Materials Science and Enginnering (CALPHAD, DICTRA, Micress, Abaqus, LS-Dyna, LAMMPS, etc.).
In-house developed codes

**IRIS ©**

IRIS is an object oriented, general purpose, parallel code for computational mechanics in solid, fluid, and structural applications. It has finite element and meshless capabilities, a wide range of material models, and solvers for linear and nonlinear, stationary and transient simulations. Currently, it can be applied in problems of linear and nonlinear solid mechanics, beams, shells, membranes, compressible and incompressible flows, thermal analysis and thermomechanical problems.

**CAPSUL ©**

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

- A crystal plasticity constitutive model, aimed at predicting the elasto-plastic behaviour at the crystal level. The model incorporates physically-based and phenomenological implementations and both slip and twinning mechanisms are considered. Both monotonic response and cyclic behaviour are considered by the combination of different laws for isotropic hardening, kinematic hardening and cyclic softening. The model has already been successfully applied to simulate the mechanical performance of FCC (Al and Ni-based superalloys) and HCP alloys (Mg and Ti), including stress-strain curves and texture evolution under monotonic loading as well as crack initiation and fatigue life under cyclic loading. The model is programmed as a UMAT subroutine for Abaqus.

- A tool to generate finite element models representative of the actual alloy microstructure (grain size, shape and orientation distribution) using as input statistical data obtained from microscopy images.

- An inverse optimization tool to obtain the crystal plasticity model parameters from the result of a set of mechanical tests (both microtests or tests on polycrystals).

- A set of python scripts to generate cyclic loading conditions and to postprocess the results to obtain fatigue indicator parameters and other measures from microfields.
VIPER ©

VIPER is a simulation tool developed within the framework of computational micromechanics 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.

Muesli ©

MUESLI is an Open Source library of material models for general numerical methods of continuum mechanics problems. It includes common models for elastic and inelastic solids in small and large strain regimes (elastic, J2 plastic, viscoelastic, Ogden, Neo-hoohean, Mooney-Rivlin, …) as well as the standard fluid materials (Newtonian and non-newtonian). Written in C++, it has been designed for easy integration with existing research codes and extensibility. In addition, an interface with LS-Dyna and Abaqus is provided so that the implemented material models can be used, without modification, in these commercial finite element codes.

MMonCa ©

MMONCA is an 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.

For more information about IMDEA Materials Institute’s codes visit http://www.materials.imdea.org/research/software.
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 0° to 60°, heavy duty downdraft bench (AirBench FP126784X) and turret milling machine (LAGUN FTV-1).
current research projects

annual report
2015
During 2015, the Institute has participated in 68 research projects, 17 of which began during the year. With respect to project funding, 2015 experienced a year-on-year increase of 5%. In particular, project funding coming from European projects and industrial contracts was similar compared to year 2014, whereas funding coming from national and regional competitive calls increased by 148% year-on-year.

The project portfolio is divided into three main groups: 32 projects were obtained in international competitive calls, out of which 17 were funded by the European Union, 12 by the Chinese Scholarship Council, one 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 two projects were funded by the Russian Federation and CAPE Foundation of Brazil, respectively. In addition, 11 projects were supported by research programmes sponsored by MINECO and two by the Regional Government of Madrid, while 23 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 2015 by funding source
A brief description of the projects started in 2015 is provided below:

**VIRMETAL**

“Virtual design, processing and testing of advanced metallic alloys for engineering applications”

Funding: European Research Council, European Union-Horizon 2020 Programme  
Duration: 2015-2020  
Principal Investigator: Prof. J. Llorca

The project VIRMETAL is aimed at developing multiscale modelling strategies to carry out virtual design, virtual processing and virtual testing of advanced metallic alloys for engineering applications so new materials can be designed, tested and optimized before they are actually manufactured in the laboratory. The focus of the project is on materials engineering i.e. understanding how the structure of the materials develops during processing (virtual processing), the relationship between this structure and the properties (virtual testing) and how to select materials for a given application (virtual design). Multiscale modelling is tackled using a bottom-up, hierarchical, modelling approach. Modelling efforts will begin with ab initio simulations and bridging of the length and
time scales will be accomplished through different multiscale strategies which will encompass the whole range of length and time scales required by virtual design, virtual processing and virtual testing. Nevertheless, not everything can or should be computed and critical experiments are an integral part of the research program for the calibration and validation of the multiscale strategies.

The research is focused on two cast metallic alloys from the Al-Cu-Mg and Mg-Al-Zn systems to demonstrate that the structure and properties of two standard engineering alloys of considerable industrial interest can be obtained from first principles by bridging a cascade of modelling tools at the different length scales. Once this is proven, further research will lead to the continuous expansion of both the number and the capability of multiscale simulation tools, leading to widespread application of Computational Materials Engineering in academia and industry. This will foster the implementation of this new revolutionary technology in leading European industries from aerospace, automotive, rail transport, energy generation and engineering sectors.
COMETAD
“Development of computational and experimental techniques for analysis and design of fire retardant polymers”

Funding: National programme for the promotion of excellence in scientific and technical research, Spanish Ministry of Innovation and Competitiveness

Partners: International Center for Numerical Methods in Engineering (CIMNE), Project Coordinator) and IMDEA Materials Institute

Duration: 2015-2017

Principal Investigator: Dr. D. Y. Wang

Flammability of polymer-based materials is a serious hazard for society. Improving the fire retardancy of polymeric materials by means of additives without compromising other properties is necessary to expand their use in many industrial applications. Within this framework, the objectives of COMETAD project are the following: i) to understand the physical mechanisms that enhance the fire resistance in polymers containing flame-retardant additives, ii) to incorporate these mechanisms into a multiphysics numerical tool. The new tool will be validated against fire test at the laboratory scale and, iii) to design (guided by the new tool) and manufacture the next generation of eco-friendly flame retardant additives.
**FUTURALVE**

“Materials and advanced fabrication technologies for the new generation of high speed turbines”

**Funding:** Centre for Industrial Technological Development (CIEN programme), Spanish Ministry of Economy and Competitiveness and Industria de Turbo Propulsores S.A. (ITP)

**Partners:** National consortium led by ITP. IMDEA Materials Institute collaborates with ITP.

**Duration:** 2015-2016

**Principal Researchers:** Dr. J. Molina and Dr. I. Sabirov

FUTURALVE is a national R&D collaborative program carried out by a consortium of companies and led by ITP. The goal of the project is to create new materials and advanced fabrication technologies for the new generation of high speed turbines.

IMDEA Materials’ activities are mainly focused on the analysis of cracking susceptibility during solidification and the characterisation of residual stresses, microstructure and defectology. The research activities are performed by an interdisciplinary team including researchers from the Physical Simulation, Micro- and Nano-Mechanics and X-Ray Characterisation of Materials research groups.

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**STEM**

“Structural energy harvesting composite materials”

**Funding:** Projects Europe Excellence, Spanish Ministry of Economy and Competitiveness

**Duration:** 2015-2016

**Principal Investigator:** Dr. J. J. Vilatela

The purpose of this project is to build the fundamentals towards the development of new multifunctional structural composite materials that combine high-performance mechanical properties and the possibility to harvest energy. The uniqueness of this project lies in exploiting advanced optoelectronic processes in macroscopic strong composites on a composite ply length-scale, in the quest for a new generation of light-weight multifunctional structural materials.
**MICROFRAC**

“Visualization and modeling of fracture at the microscale”

**Funding:** Marie Skłodowska-Curie-IF, European Union-Horizon 2020 Programme  
**Duration:** 2015-2016  
**Principal Investigator:** Dr. A. Weck

MicroFrac aims at providing a significant contribution towards our understanding of fracture at the microscale through a combination of state-of-the-art experiments and models. Micro voids will be introduced in metallic single crystals and their growth will be followed in-situ at high resolution. The effects of void size and crystal orientation will be investigated and the results will be used to validate dislocation dynamics and crystal plasticity models of void growth.

The expected outcomes of the project will be new experimental evidence of fracture at the microscale and the creation of an improved crystal plasticity model that can take into account size effects during void growth to improve the predictions of ductile fracture by nucleation, growth and coalescence of voids. New material designs with improved fracture resistance will also be proposed.

**ADVANSEAT**

“Modular concept for ultralight removable advanced car seat”

**Funding:** Centre for Industrial Technological Development (CIEN programme), Spanish Ministry of Economy and Competitiveness and Grupo Antolin  
**Partners:** National consortium led by Grupo Antolin. IMDEA Materials Institute collaborates with Grupo Antolin.  
**Duration:** 2015-2017  
**Principal Researchers:** Dr. C. González and Dr. C. S. Lopes
This collaborative R&D project, led by Grupo Antolín with the participation of other companies from the automotive sector, aims at developing a new modular concept of advanced seat, removable, with ultralight structure obtained by more efficient and flexible transformation process, and with electrification for security and comfort functions.

The main role of IMDEA Materials’ team in the project is to develop a physically based numerical methodology based on the finite element method to analyse the mechanical behaviour of the seat materials. The final aim is to use and integrate the model into a commercial finite element code to analyse dynamic loadings.

**NEOADFOAM**

“Innovative additives for foams with improved thermal insulation and fire resistance”

*Funding:* Challenges - Collaboration, Spanish Ministry of Innovation and Competitiveness  
*Partners:* TOLSA S.A. (Project Coordinator), Cellmat group (University of Valladolid) and IMDEA Materials Institute  
*Duration:* 2015-2017  
*Principal Investigator:* Dr. D. Y. Wang

The main objective of this research project funded by MINECO is to develop a family of multifunctional additives for polymeric foams. Those additives will be based on the combination of functionalised nanosepiolites with other active elements capable of improving, at the same time, the thermal insulation, mechanical and fire resistance properties of the foams under study. NEOADFOAM project will focus on two materials widely employed as thermal insulators in the construction industry: expanded polystyrene and rigid polyurethane foams. The solutions that will be developed aim to provide turnkey answers to foam producers (target market) in order to improve the added value of their products.
HIPREP
“High Performance Reinforced Fire-retardant Polymers”

Funding: China Scholarship Council
Duration: 2015-2019
Principal Researchers: Dr. D. Y. Wang

The objective of this investigation is to develop high performance reinforced fire-retardant polymers via special molecular design, chemical functionalization of the reinforced fibers and advanced polymer processing. The fire behaviours, mechanical properties, interfacial properties and thermal properties will be systematically studied.

TK-Cobalt
“High Throughput Diffusion Experimentation and Computational Thermo-Kinetics for Advanced Co-base High Temperature Alloys”

Funding: China Scholarship Council
Duration: 2015-2019
Principal Researchers: Dr. Y. Cui and Prof. J. LLorca

The research, with a focus on the Co-base high temperature alloys, aims at developing a robust high throughput diffusion couple technique. The new technique will enable fast mapping of such information as phase diagram, diffusion coefficient and transformation kinetics, which will be in turn acted as combinatorial experimental platform for new advanced alloy design.
MICROTEST
“Correlation study of mechanical properties / microstructure / fracture behaviour of industrial parts and standardized tensile specimens”

Funding: European Powder Metallurgy Association (EPMA)
Duration: 2015-2016
Principal Researchers: Dr. T. Pérez-Prado

MicroTest is an R&D project with European Powder Metallurgy Association (EPMA) to study the mechanical properties and the fracture behaviour in correlation with the microstructure using real parts and specimens produced in industrial conditions.

DOPANTSPER
“Physical modeling of electrical junctions based on low temperature process flow”

Funding: ST Microelectronics
Partners: ST Microelectronics, Commissariat à l’Energie Atomique et aux Energies Alternatives (CEA) and IMDEA Materials Institute
Duration: 2015-2017
Principal Researchers: Dr. I. Martin Bragado

The main goal of this research work will be to study the physical mechanisms and their impacts on the electrical performance of microelectronic devices in a fully integrated simulation platform. The developed models and simulation tools will contribute to the optimization of microelectronic devices in low temperature process integration schemes.
**OKMC4III-V**

“Diffusion and activation of dopants and Impurities in InGaAs”

**Funding:** GlobalFoundries Singapore  
**Partners:** GlobalFoundries Singapore, Nanyang Technological University (NTU) and IMDEA Materials Institute  
**Duration:** 2015-2017  
**Principal Researchers:** Dr. I. Martin Bragado

Collaborative research project with NTU and the company GlobalFoundries to develop advanced simulation tools to optimise diffusion and activation of dopants and impurities in InGaAs.

**NearBetaTi**

“Structural phase transformation under shear and composition gradient in Ti alloys”

**Funding:** China Scholarship Council  
**Duration:** 2015-2019  
**Principal Researchers:** Dr. Y. Cui and Dr. J. Molina

The project is firstly aimed at processing the selected near β Ti alloy by high pressure torsion, characterizing the grain size and phase distribution of the resulting microstructures and measuring their mechanical behaviour. In addition, the development of phase transformations in near β Ti (including Ti-5553) will be analyzed by the high throughput diffusion multiple approach.

**CRIRCEM**

“Development of innovative materials for the cutting tool industry”

**Funding:** China Scholarship Council  
**Duration:** 2015-2019  
**Principal Researchers:** Dr. A. García-Junceda
This investigation proposes the design and processing by powder metallurgical routes of new materials for cutting tools with total substitution of the traditional cobalt binder by other more economic and less toxic. These innovative materials will combine all the requirements needed in the tool materials industry, such as: high elastic modulus, high hardness, strength, abrasion resistance, mechanical impact strength, compressive strength, thermal shock resistance and corrosion resistance.

CRISTAL
“Corrosion resistant Zn-Al hypoeutectic alloys”

Funding: CAPES Foundation, Brazil
Duration: 2015 - 2016
Principal Researchers: Dr. S. Milenkovic

Zn-Al alloys are widely applied in different engineering applications where the superior wear and corrosion resistance are required. Cu and Mg are often added to further improve their properties. Although Cu has an important influence on the properties of Zn-Al alloys, the presence of the metastable phase epsilon (CuZn4, intermetallic compound) may cause dimensional instability of the alloy over time due to its transformation into the stable pi phase. The formation of metastable phase CuZn4 and the associated phase transformations by heat treatments have been studied for eutectic and hypereutectic Zn-Al, alloys, but there is little information reported in the literature on these changes for Zn-Al hypoeutectics alloys.

The main objective of CRISTAL project is to improve corrosion resistance of commercial Zamac 8 alloy (Zn-4Al-2,6Cu-0,5Mg) by microstructure control which will be achieved by varying the Cu content, the solidification rate, heat treatments and the combination of thereof.
**EXTRECP**

“Crystal Plasticity modeling under extreme conditions”

Funding: China Scholarship Council  
Duration: 2015-2019  
Principal Researchers: Dr. J. Segurado and Prof. I. Romero

The goal of this research is the development of coupled thermomechanical crystal plasticity models to simulate problems under extreme conditions: very large strain rates and high temperatures.

Firstly, the effect of strain rate and temperature will be introduced in the crystal plasticity model through the use of physically based models. The basis of these studies is the thermally activated character of many deformation mechanisms: dislocation nucleation, slip, cross slip and other short-range interactions. Secondly, a strong thermo-mechanical coupling framework will be proposed at the crystal level. The aim here is to extend the present modelling approaches to include thermal strains, thermally dependent plastic behaviour and the ability to account for high strain rates. This framework will contain most of the details necessary for simulating processes under extreme conditions such as machining, impact, etc.

**FIREINF**

“Fire retardant epoxy infusion resin composites”

Funding: Foundation for the Research Development and Application of Composite Materials (FIDAMC)  
Partners: Foundation for the Research Development and Application of Composite Materials (FIDAMC) and IMDEA Materials  
Duration: 2015-2016  
Principal Researchers: Dr. D. Y. Wang
Research collaboration between IMDEA Materials Institute and FIDAMC with the goal of developing an effective novel halogen-free fire retardant epoxy system to be used in out-of-autoclave processes to manufacture composite components/structures. This fire-retardant epoxy resin will be applicable to any industrial sector with strict fire smoke toxicity requirements such as aeronautics, automotive or railway.

Other ongoing research projects in 2015 at IMDEA Materials Institute were:

**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

**DESMAN “New structural materials for energy harvesting and storage”**

Funding: B/E Aerospace Inc (USA)  
Partners: IMDEA Energy Institute  
Duration: 2014-2017  
Principal Investigator: Dr. J. J. Vilatela
MODENA “Modelling of morphology development of micro- and nano structures”

Funding: NMP, European Union-7th Framework Programme
Partners: Norwegian University of Science and Technology (Coordinator, Norway), University of Trieste (Italy), BASF SE (Germany), Politecnico di Torino (Italy), Wikki Ltd. (UK), Eindhoven University of Technology (Netherlands), IMDEA Materials Institute (Spain), University of Stuttgart (Germany), Vysolka Skola Chemicko-Technologica (Czech Republic), Deutsches Institut für Normung (Germany)
Duration: 2013-2015
Principal Investigator: Prof. J. LLorca

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

SIMUFOING “Development and validation of simulation methods for ice and bird ingestion in plane engines”

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

NEW EPOXY “New generation high-performance fire retardant epoxy nanocomposites: structure-property relationship”

Funding: Marie Curie Action - IIF, European Union-7th Framework Programme
Duration: 2014-2016
Principal Investigator: Dr. Jin Tao Wan and Dr. D. Y. Wang
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

VIRTEST “Multiscale virtual testing of CFRP samples”

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

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

Funding: Centre for Industrial Technological Development (CIEN programme), Spanish Ministry of Economy and Competitiveness and Industria de Turbo Propulsores S.A. (ITP)
Duration: 2014-2015
Principal Investigators: Dr. F. Sket and Dr. J. Molina

EPISIM “Simulation of epitaxial growth”

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

ONLINE-RTM “Online NDT RTM inspection in composites”

Funding: Centre for Industrial Technological Development (ESTENEA CIEN programme), Spanish Ministry of Economy and Competitiveness and Airbus Operations S.L.
Duration: 2014-2015
Principal Investigator: Dr. C. Gonzalez
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 (UPM), Department of Materials Science, Technical University of Madrid (UPM), Carlos III University of Madrid and Complutense University of Madrid.
Duration: 2013-2017
Principal Investigator: Dr. M. T. Perez-Prado

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: 2013-2017
Principal Investigators: Dr. J. J. Vilatela and Dr. J. Molina

FERROGENESYS “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

SEPIFIRE “Study of sepiolite-based fire retardant systems”

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
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), Characterisation 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

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

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

CUCCOMP “Development of Cu-C metal matrix composites”

Funding: China Scholarship Council
Duration: 2014-2015
Principal Investigator: Prof. J. M. Torralba
MATERPLAT “Spanish technology platform of advanced materials and nanomaterials”
Funding: Spanish Ministry of Economy and Competitiveness
Duration: 2014-2015
Project Responsible: M. A. Rodiel

MICROMECH “Microstructure based material mechanical models for superalloys”
Funding: Clean Sky Joint Undertaking, EU Seventh Framework Programme for Research (FP7)
Partners: IMDEA Materials Institute
Duration: 2013-2015
Principal Researcher: Dr. J. Segurado

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), INAES 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
**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 (Ireland), 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:** 2013-2016  
**Principal Investigator:** Dr. J. J. Vilatela and Dr. J. P. Fernández

**ICMEG “Integrative computational materials engineering expert group”**

**Funding:** NMP, European Union-7th Framework Programme  
**Partners:** ACCESS e.V. (Germany), K&S GmbH Projektmanagement (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: 2013-2015
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: 2012-2015
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: 2012-2016
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: 2012-2015
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: 2012-2015
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

MODELQP “Ginzburg-Landau model for the mixed microstructure in new Q&P steels”
Funding: China Scholarship Council (China)
Duration: 2011-2015
Principal Investigators: Dr. Y. Cui and Prof. J. LLorca

MASID “Modelling of advanced semiconductor integrated devices
Funding: Global Foundries Singapore Pte Ltd. (Singapore)
Duration: 2011-2015
Principal Investigator: Dr. I. Martin-Bragado
DECOMP “Development of advanced ecofriendly polymer nanocomposites with multifunctional properties”

Funding: China Scholarship Council (China)
Duration: 2011-2015
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: 2010-2015
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: 2008-2015
Principal Investigator: Dr. C. González
dissemination of results

6.1. Publications [79]
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6.1. Publications


spectromicroscopy: towards near-ambient-pressure experiments, CHEM CATCH 7, 3665-3673, 2015.


59. M. Rahimian, S. Milenkovic, L. Maestro, A. Eguidazu Ruiz De Azua, I. Sabirov, Development of tool for physical simulation of skin forma-


73. I. Martín-Bragado, J. Abujas, P. L. Galindo, J. Pizarro, Synchronous parallel Kinetic Monte Carlo: Implementation and results for object and lattice approaches, Nuclear Instruments and Methods in Physics Research Section B: Beam Inte-


6.2. Book Chapters


6.3. Patents


6.4. License Agreements

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

6.5. International Conferences

Invited and Plenary talks


17. “Nanostructuring in Aluminium alloys for improvement of their mechanical and functional properties”, I. Sabirov, M. Murashkin, R. Z. Valiev, XXIV International Materials Research Congress, Cancun, Mexico, August 2015.


Regular Contributions


47. “Multiscale characterization strategy for the microstructure and the mechanical properties of polyurethane foams”, M. Marvi-Mashhadi, C. S.


82. “Anomalous high temperature strengthening of Mg-RE alloys”, P. Hidalgo-Manrique, F. Carreño, D. Letzig, M. T. Pérez-Prado, European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2015), Warsaw, Poland, September 2015.


85. “Carbon nanotube/inorganic hybrids for energy harvesting”, A. Monreal, J. J. Vilatela, European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2015), Warsaw, Poland, September 2015.

86. “Synthesis of kilometers of continuous macroscopic fibres with controlled type of CNTs and bundle orientation”, V. Reguero, B. Alemán, B. Mas, J. J. Vilatela, European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2015), Warsaw, Poland, September 2015.


106. “Influence of copper addition, solidification rate and heat treatments on the microstructure and hardness of Zn-Al hypoeutectic alloys”, R. Sanguiné, E. Costa, S. Milenkovic,
T. Batistella, Advances in Materials and Processing Technologies Conference 2015 (AMPT 2015), Leganés, Spain, December 2015.


Membership in Organising Committees


8. International Conference of Composite Materials (ICCM20). C. González (Coordinator of Track 3-7: Models Homogenization – Micro to Macro-Effective properties, intact and damaged materials, multi-scale modelling, representative-Volume-Element (RVE), and Member of the Scientific Committee). Copenhagen, Denmark, July 2015.

10. **17th International Conference on the Strength of Materials (ICSMA 17)**. M. T. Pérez-Prado (Member of the International Advisory Board). Brno, Czech Republic, August 2015.


12. **12th International Conference on Superplasticity in Advanced Materials (ICSAM 2015)**. M. T. Pérez-Prado (Member of the International Advisory Board). Tokyo, Japan, September 2015.


17. **Congreso Internacional de Materiales (CIM 2015)**. J. M. Torralba (Member of the International Scientific Committee). Paipa, Colombia, October 2015.


22. **Advances in Materials and Processing Technologies Conference 2015 (AMPT 2015)**. S. Milenkovic (Co-organizer of the Symposium on Frontiers of Intermetallics and Member of the Local Organizing Committee). Leganés, Spain, December 2015.
6.6. Organisation of International Conferences and Workshops

Three international workshops and two international conferences were organised by IMDEA Materials Institute in 2015. The Workshops were held at the Institute, taking advantage of the facilities available in our building, and the conferences took place in the University Carlos III of Leganes. Over 1600 delegates attended these events, enhancing the international visibility of our activities.

Other important events held at the Institute was the “I IMDEA Conference: Science, Business and Society” organized by all the IMDEA Institutes with more than 500 participants. The conference counted with the presence of Mrs. Cristina Cifuentes, President of the Madrid regional government (Comunidad de Madrid).


2. 7th International Conference on Composites Testing and Model Identification, C. Gonzalez and C. Lopes (Chairmen), April 2015

3. 9th European Solid Mechanics Conference, J. LLorca (Chairman), July 2015

4. I IMDEA Conference: Science, Business and Society, Organized by all the IMDEA Institutes, November 2015

5. 1st Workshop on Nanostructured Materials for Light Harvesting Technologies, J. J. Vilatela (Chairman), November 2015


Figure 6. I IMDEA Conference opening session speakers. From left to right, Fernando Temprano, Javier LLorca, Fernando Suárez, Cristina Cifuentes, Carmen Vela, Rafael van Grieken and Guillermo Reglero
6.7. Invited Seminars and Lectures


6. “Application of physical simulation for development of complex SPD processing routes”. I. Sabirov, Institute of High Pressure Physics, Polish Academy of Sciences, Celestynów, Poland, June 2015.


12. “Diffusion fundamentals and applications”. Y. Cui, Nanjing Technical University, Nanjing, China, June 2015.


15. “Is halogen-free fire retardant low efficient?”. D. Y. Wang, Anhui University of Science and Technology, Huainan City, China, July 2015.


29. “Multiscale Virtual Testing: The roadmap to the efficient design of composites for structural
6.8. Seminars

1. “Experimental –numerical dialog in the FEMME (Finite Element model with a Micr
structural adaptive MEshfree framework) multiscale fracture model”, Dr. Luis Saucedo (from Oxford University). January 2015.


15. “Carbon nanotube - inorganic hybrids: from synthesis to application”, Dr. Laura Cabana (from Universidad Autónoma de Barcelona). September 2015.


17. “To wet or not to wet. Liquid-repellent coatings”, Dr. Noemí Encinas (from Max Planck Institute for Polymer Research). October 2015.


6.9. Fellowships

1. Marie Skłodowska-Curie-Individual Fellowship (IF), European Union, Horizon 2020 Programme
   - Call 2014: Dr. A. Weck

2. Marie Curie-International Incoming Fellowship (IIF), European Union, 7th Framework Programme
   - Call 2013: Dr. Jintao Wan

3. AMAROUT EUROPE Programmes (I and II), Marie Curie Action (PEOPLE-COFUND), European Union, 7th Framework Programme
   - Call 2015: Dr. M. Haranczyk, Dr. A. Moitra
   - 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. Babluena
   - 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. Raja-kesari, Dr. S. R. Bonta
   - Call 2009: Dr. R. Seltzer, Dr. I. Sabirov, Dr. A. Jerusalem

4. Ramon y Cajal Programme, Spanish Ministry of Economy and Competitiveness
   - Call 2014: Dr. J. J. Villatela
   - 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

5. Fullbright Secondment, Spanish Ministry of Education, Culture and Sport
   - Call 2014: Dr. J. Molina

6. Postdoctoral Fellowship Programmes, Spanish Ministry of Economy and Competitiveness
   - Call 2013: Dr. F. Sket
   - Call 2012: Dr. H.-J. Chang
6.10. Awards

1. 2014 Zwick Science Award
   · Dr. Rocío Muñoz

   · Dr. Raúl Muñoz

3. 2015 APMI Fellow Award, American Powder Metallurgy Institute (APMI)
   · Prof. José Manuel Torralba

4. 2015 Young Academics’ European Steel Award, Association of German Steel Manufacturers (VDEh)
   · Dr. I. De Diego-Calderon

5. 2015 Outstanding PhD Thesis Award, Carlos III University of Madrid
   · Dr. M. Rahimian

6. Honourable Mention to the Public-Private Cooperation with exploitable research results, X Madri+d Awards
   · Dr. C. González and Dr. C. Lopes

7. Excellence in Metallography Award, POWDER-MET2015 Conference
   · Prof. J. M. Torralba

8. 2015 Fulbright Scholarship, The F. William Fulbright Foreign Scholarship Board and the Bureau of Education and Culture of the United States Department of State and the Spanish Ministry of Education and Culture
   · Dr. J. M. Molina-Aldareguia

9. 2015 Stiftelsen för Tillämpad Termodynamik grant 2015, Foundation for Applied Thermodynamics
   · G. Xu
6.11. Institutional Activities

- Member of the European Materials Modelling Council (EMMC)
- Member of the European Energy Research Alliance (EERA AISBL)
- Member of the Technical Committee of the M-Eranet promoted and funded by the European Commission
- Member of the European Composites, Plastics and Polymer Processing Platform (ECP4)
- Member of the Board of Directors of the Spanish Association of Composite Materials (AEMAC)
- Coordinator and member of the Management Board 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 Aerospace, 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 Madrid.
- Participation in the European Researchers’ night Madrid 2015, promoted by Fundación Madrid.

6.12. Theses

6.12.1. PhD Theses

“Physical simulation of investment casting of Mar-M247 Ni-based superalloy”  
Student: Mehdi Rahimian  
Carlos III University of Madrid  
Advisor: Dr. I. Sabirov and Dr. S. Milenkovik  
Date: July 2015

“Mechanical properties of advanced high-strength steels produced via Quenching and Partitioning”  
Student: Irene de Diego  
Carlos III University of Madrid  
Advisors: Dr. I. Sabirov and Dr. J. M. Molina-Aldareguia  
Date: September 2015

“Polymer interaction with macroscopic carbon nanotube fibres and fabrication of nanostructured composites”  
Student: Hangbo Yue  
Technical University of Madrid  
Advisors: Dr. J. J. Vilatela and Prof. J. LLorca  
Date: September 2015

6.12.2. Master/Bachelor Theses

“Tratamiento de imágenes para cuantificación del daño en volúmenes de tomografía en 4D de CFRP [±45]2S”  
Student: Antón Jormescu  
Technical University of Madrid  
Advisor: Dr. F. Sket  
Date: January 2015

“Músculo Artificial basado en polímero electroactivo”  
Student: Juan Carlos Rubalcaba  
Carlos III University of Madrid  
Advisor: Dr. R. Guzmán de Villoria  
Date: March 2015
“Time multiscale models for the simulation of slow transport problems in atomistic systems”
Student: Borja González
Technical University of Madrid
Advisor: Dr. I. Romero
Date: June 2015

“Relationship between internal porosity and fracture strength of Ni-based alloys”
Student: Bogdan Nedelcu
Carlos III University of Madrid
Advisor: Dr. F. Sket
Date: July 2015

“Influencia del procesado de torsión a alta presión sobre la microestructura y las propiedades mecánicas de la aleación de aluminio AA6082”
Student: Miriam Gómez
Technical University of Madrid
Advisor: Dr. C. Cepeda
Date: July 2015

“Flame retardants with phosphorous compounds on epoxy resins”
Student: Francisco Hueto
Technical University of Madrid
Advisor: Dr. D. Wang
Date: July 2015

“Estudio del proceso de recristalización epitaxial en fase sólida de aleaciones de silicio-germanio para aplicaciones microelectrónicas espaciales mediante Dinámica Molecular”
Student: David Sierra
Technical University of Madrid
Advisor: Dr. I. Martín Bragado
Date: July 2015

“Formability of Cu alloys after severe plastic deformation”
Student: Pedro Asenjo
Carlos III University of Madrid
Advisor: Dr. I. Sabirov
Date: July 2015

“Estudio de la conformabilidad de la aleación de Magnesio MN11”
Student: Víctor Coiradas
Technical University of Madrid
Advisor: Dr. P. Hidalgo
Date: July 2015

“Electrochemical delamination of CVD-grown transparent and electrical conductive carbon film”
Student: Cristina Diego
Technical University of Madrid
Advisor: Dr. R. Gúzman de Villoria
Date: July 2015

“Ionic polymer-metal composites: manufacturing and characterization, aeronautical engineering”
Student: Clara Andrea Pereira
Carlos III University of Madrid
Advisor: Dr. R. Gúzman de Villoria
Date: July 2015

“Synthesis, fabrication, mechanical and electrical characterization of alumina nanoparticles/carbon nanotube epoxy composites”
Student: Jaime Tortosa
Rey Juan Carlos University
Advisor: Dr. R. Gúzman de Villoria
Date: July 2015

“Automation of the pre- and post-processing of the simulation of micropillar compression tests by python scripting (Abaqus)”
Student: Álvaro Corbato
Technical University of Madrid
Advisor: R. Sánchez
Date: July 2015

“Design and preparation of flame retardant PP composites via thermal compounding”
Student: Sergio de Juan
Carlos III University of Madrid
Advisor: Dr. D. Wang
Date: July 2015
“Microstructure and phase equilibrium of the NiAl-Cr-W and NiAl-Cr-Re pseudo-ternary systems. Characterisation of the eutectic trough”
Student: Álvaro Menduiña
Technical University of Madrid
Advisor: Dr. S. Milenkovic
Date: July 2015

“Microestructura y comportamiento mecánico de Cu puro laminado, trefilado y extruido”
Student: Mario Antón
Carlos III University of Madrid
Advisor: Dr. T. Pérez Prado
Date: July 2015

“Microstructural design in TiAl with high cooling rates via dynamic plastic deformation and quenching”
Student: Raúl García
Carlos III University of Madrid
Advisor: Dr. T. Pérez Prado and Dr. I. Sabirov
Date: July 2015

“Tomographic Investigation of sequential tensile loading of [±45]2s Carbon Fiber Laminates”
Student: Héctor Alcoceba
Technical University of Madrid
Advisor: Dr. F. Sket
Date: September 2015

“Evaluation of damage mechanisms during tensile and fatigue test of AZ31 Mg alloy by means of synchrotron X-ray microtomography”
Student: Guillermo Centelles
Technical University of Madrid
Advisor: Dr. F. Sket
Date: September 2015

“Diseño y caracterización de aceros inoxidables dúplex consolidados mediante la técnica de compactación en caliente asistida por campo eléctrico (Field Assisted Hot Pressing, FAHP)”
Student: María Rincón
Carlos III University of Madrid
Advisor: Dr. A. García-Junceda and Prof. J. M. Torralba
Date: October 2015

“Diseño de un nuevo carburo cementado de matriz base Cr-Fe”
Student: Israel Sáez
Carlos III University of Madrid
Advisor: Dr. A. García-Junceda and Prof. J. M. Torralba
Date: October 2015

“Behaviour of previously delaminated composite plates under ballistic impact”
Student: Raquel Álvarez
Technical University of Madrid
Advisor: V. Martínez and Prof. C. González
Date: October 2015

“Effect of copper surface state during glass-like carbon synthesis”
Student: Hugo Mora
Carlos III University of Madrid
Advisor: Dr. R. Gúzman de Villoria
Date: November 2015
6.13. Internships / Visiting Students

“Characterization, design and optimization of dispersed-ply laminates”
Student: Peyman Mouri
Date: August 2014-July 2015
Advisor: Dr. C. Lopes
Visiting student from: Delft University of Technology. The Netherlands

“Buckling and failure optimization of stiffened tow-steered composite panels”
Student: Momchil Jeliazkov
Date: August 2014-August 2015
Advisor: Dr. C. Lopes
Visiting student from: Delft University of Technology. The Netherlands

“Microstructure and properties of SPD processed Cu alloys”
Student: Ivan Lomakin
Date: January 2015-December 2015
Advisor: Dr. I. Sabirov
Visiting student from: Saint-Petersburg State University. Russia

“Flame retardant and mechanical properties of natural fibers reinforced polymer”
Student: Mohammad Rajaei
Date: January 2015-March 2015
Advisor: Dr. D. Wang
Visiting student from: University Oakland. New Zealand

“Polymer Nanocomposites”
Student: Xuanliang Zhao
Date: February 2015-May 2015
Advisor: Dr. D. Wang
Visiting student from: Beihang University. China

“Chemical synthesis & bench scale fire testing”
Student: Anabel Montes
Date: March 2015-May 2015
Advisor: Dr. D. Wang
Visiting student from: Rey Juan Carlos University. Spain

“Mechanical behaviour of glass fiber nonwoven networks”
Student: Ying-Long Chen
Date: April 2015-June 2015
Advisor: Prof. J. Llorca and Dr. C. González
Visiting student from: School of Mechanical Engineering, Purdue University. United States of America

“Computational Micromechanics of Recycled Composites”
Student: Bo-Cheng Jin
Date: April 2015-August 2015
Advisor: Prof. J. Llorca and Dr. C. González
Visiting student from: Southern California University. United States of America

“Tensile properties of CNT fibres”
Student: Damien Eustache
Date: May 2015-August 2015
Advisor: Dr. J. J. Vilatela
Visiting student from: Polytech Montpellier. France

“Strain rate sensitivity of Zr-based bulk metallic glasses subjected to high pressure torsion”
Student: Boltyniuk Evgenii
Date: May 2015-December 2015
Advisor: Dr. I. Sabirov
Visiting student from: St. Petersburg State University. Russia

“Analysis of internal damage evolution in steels with different fracture behaviour”
Student: Rachel Shifman
Date: May 2015-August 2015
Advisor: Dr. F. Sket
Visiting student from: Michigan State University. United States of America

“Hot rolling of Mg alloys using Gleeble technology”
Student: Isabel Arauz de Robles
Date: May 2015-July 2015
Advisor: Dr. C. Cepeda
Visiting student from: Polytechnique Montreal. France
“High Performance Polymer Nanocomposites”
Student: François Dufosse
Date: July 2015-September 2015
Advisor: Dr. D. Wang
Visiting student from: ENSCL Chimie Lille, France

“Transport properties of CNT fibres”
Student: Agustín Iñiguez
Date: June 2015-August 2015
Advisor: Dr. J. J. Vilatela
Visiting student from: TuDELFT, The Netherlands

“Direct evaluation of fracture toughness in carbon, glass and aramid fibres with an artificial notch introduced by focused-ion-beam”
Student: Andrea Fernández
Date: June 2015-September 2015
Advisor: M. Herráez, Dr. C. S. Lopes and Dr. C. González
Visiting student from: Polytechnical University of Gijon, Spain

“Synthesis of CNT/MOx hybrids”
Student: Jorge González
Date: June 2015-August 2015
Advisor: Dr. J. J. Vilatela
Visiting student from: Alicante University, Spain

“Bioinspired hierarchical composites: Mechanical characterization of composite laminates”
Student: Carlos Vasquez
Date: May 2015-October 2015
Advisor: Dr. R. Guzmán de Villoria
Visiting student from: Technical University of Madrid, Spain

“Experimental characterization of the intralaminar mechanical properties of discontinuous directional composites”
Student: María Castillo
Date: May 2015-October 2015
Advisor: Dr. R. Guzmán de Villoria
Visiting student from: Technical University of Madrid, Spain

“Formability of quenched and partitioned steels.”
Student: Miguel A. Valdés
Date: June 2015-September 2015
Advisor: Dr. I. Sabirov
Visiting student from: Technical University of Madrid, Spain

“Research Initiation Fellowship”
Student: Rebeca Muñoz
Date: July 2015-September 2015
Advisor: Dr. I. Romero
Visiting student from: Technical University of Madrid, Spain

“PVC Nanocomposites”
Student: Víctor Alelu
Date: September 2015
Advisor: Dr. D. Wang
Visiting student from: Autonomous University of Madrid, Spain

“Flame retardant poly (lactic acid) nanocomposite”
Student: Weijun Yang
Date: September 2015-December 2015
Advisor: Dr. D. Wang
Visiting student from: University of Perugia, Italy

“Experimental Characterization of Triaxially Braided Composites”
Student: Wilko Roelse
Date: September 2015-December 2015
Advisor: Dr. A. Garcia-Carpintero, Dr. C. S. Lopes and Dr. C. González
Visiting student from: Eindhoven University of Technology, The Netherlands
“Chemical Vapor Deposition”
Student: Sofía Roselló
Date: June 2015-July 2015
Advisor: Dr. R. Guzmán de Villoria
Visiting student from: Autonomous University of Madrid. Spain

“Interaction of liquids with CNTs fibres”
Student: Zaiqin Zhang
Date: January 2015-May 2015
Advisor: Dr. J. J. Vilatela
Visiting student from: Beihang University, China

“Effect of crystal orientation on void growth of pure Ti by in-situ microtomography”
Student: Marina Pushkareva
Date: April 2015-June 2015
Advisor: Dr. F. Sket
Visiting student from: University of Ottawa. Canada

“Analysis of internal damage in steel samples using X-Ray computed tomography”
Student: Samantha Schab
Date: October 2015-December 2015
Advisor: Dr. F. Sket
Visiting student from: Michigan State University. United States of America

“Fire behaviours of new flame-retardant PP composites”
Student: Xiao Dan
Date: March 2015-May 2015
Advisor: Dr. D. Wang
Visiting student from: Leibniz Institut fur Polymerforschung. Germany

“Functionalization of graphene”
Student: Xiangliang Zhao
Date: January 2015-May 2015
Advisor: Dr. D. Wang
Visiting student from: Beihang University, China

“Multifunctional composites analysis”
Student: María Barcía
Date: May 2015-October 2015
Advisor: Dr. J. J. Vilatela, J. C. Fernández and B. Mas
Visiting student from: Technical University of Madrid. Spain

“Purification and functionalization of CNTs”
Student: Daniel Iglesias
Date: August 2015-September 2015
Advisor: Dr. J. J. Vilatela and A. Moya
Visiting student from: Trieste University. Italy
6.14. 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

“Nano-Architectures and Materials Design: From Nano to Macro”
Master in Composite Materials
Technical University of Madrid and EADS
Professor: Dr. R. Guzman de Villoria

“Hierarchical composites”
Master in Composite Materials
Technical University of Madrid and EADS
Professor: Dr. J. J. Vilatela

“Simulation techniques and virtual testing”
Master in Composite Materials
Technical University of Madrid and EADS
Professors: Dr. C. González, Dr. C. S. Lopes, Dr. J. Segurado, Dr. S. Sádaba, Dr. Garijo and F. Martínez

“Metal Matrix Composites”
Master in Composite Materials
Technical University of Madrid and EADS
Professor: Dr. S. Milenkovic

“Design and Fabrication of Advanced Composite Materials”
Master in Materials Engineering
Technical University of Madrid
Professors: Prof. J. LLorca, Dr. C. González, Dr. R. Guzmán de Villoria and Dr. C. S. Lopes

“Polymeric Materials for Advanced Applications”
Master in Materials Engineering
Technical University of Madrid
Professor: Dr. D. Y. Wang

“Simulation in Materials Engineering”
Master in Materials Engineering
Technical University of Madrid
Professors: Prof. J. LLorca, Dr. I. Martín-Bragado, Dr. Y. Cui, Dr. C. González, Dr. C. S. Lopes and A. Ridruejo,

“Mechanics of composite materials”
Master in Mechanics
Saint Petersburg State University
Professor: Dr. I. Sabirov
7.1. Seeing is believing: Research programme in multiscale characterization of materials and processes [112]

7.2. Functional intercalation in LDH: Towards high performance polymer nanocomposites [118]

7.3. Computational and data-driven materials discovery [120]
Seeing is believing: Research program in multiscale characterization of materials and processes

The processing and mechanical response of any material is governed by processes that take place along several length scales (from nm to m). For instance, in the case of metals, dislocation and twin nucleation events occur at the atomic scale, dislocation-dislocation interactions extend over distances of several micrometers, and the macroscopic response is governed by the collective behavior of different grains spanning long distances. While material behavior is controlled by phenomena occurring in a single length scale in some cases (i.e., work hardening in metals), current trends to reduce weight, energy consumption and improve functionality, are leading to new materials with complex microstructures, whose behavior can only be understood from the synergetic contribution of processes occurring at multiple length scales. Examples of these materials are structural composites with a hierarchical structure, nanoporous foams and advanced metallic alloys with complex microstructures, such as nanostructured metals, duplex alloys or materials with evolving microstructures that deform by unconventional deformation mechanisms (TWIP and TRIP steels). Understanding the microstructure evolution under processing and mechanical loading of these materials is essential for future developments and this can only be attained through \textit{in-situ} or sequential methods that allow for the characterization of their microstructure (4D characterization) during processing and mechanical testing at different length scales.

The research program in Multiscale Characterization of Materials and Processes of IMDEA Materials Institute covers the activities carried out in this direction, by making use of state-of-the-art \textit{in-situ} devices (both commercial and developed in-house) to test materials under different loading configurations (tension/compression/fatigue at ambient and elevated temperature) and to simulate processing (e.g. resin infiltration of fiber preforms). Tests are carried out on specimens ranging in size from hundreds of nanometers to several millimeters under different characterization beams, such as scanning electron microscopy (SEM), focused ion beam (FIB), transmission electron microscopy (TEM), as well as X-ray computed tomography (XCT) and X-ray diffraction (XRD), both using laboratory and synchrotron X-ray radiation (http://www.materials.imdea.org/scientific-infrastructure).

Some examples of the capabilities of the program are:
Mechanical testing in the SEM and TEM at different scales (macro-micro-nano)

The behavior of wrought Inconel 718 alloys, widely used in gas turbine jet engines due to their high temperature strength, is strongly dependent on the microstructure (size and orientation of the grains, precipitate distribution, etc.). However, microstructure based models that account for the effect of the single crystal deformation of individual grains on macroscopic flow are lacking, which are critical to identify “hot spots” where damage can generate during deformation. To account for this, in situ mechanical testing in the SEM, as shown in Figure 1, can provide information on the active slip systems in each individual grain through the analysis of the slip traces observed on the surface of the specimen, and allow tracking the deformation microfields to detect these “hot spots”.

Since the macroscopic flow is determined by the plastic anisotropy at the single-crystal level, micromechanical testing is a powerful technique to develop tests capable of determining the single crystal behavior, by testing micron size specimens milled out from individual grains. For instance, Figure 2 (a) shows several micropillars of diameter 5 µm micromachined with a FIB, within individual grains of different orientations on the surface of an Inconel 718 specimen. The nanomechanical stage in Figure 2(c) allows carrying out compression experiments on these micropillars while the deformation is tracked inside a SEM at temperatures up to 800°C. Figure 2(b) shows an example for a <012> oriented micropillar where the slip traces of the two active slip systems are clearly visible. The

Figure 1. (a) Mechanical stage to carry out macrotesting in the SEM at temperatures up to 650°C. (b) Surface of an Inconel 718 specimen tested under tension showing the development of slip traces, the deformation of individual grains during deformation of the bulk material and the nucleation of microcracks.
information obtained can be used to inform single crystal plasticity models that can then be used to predict macroscopic flow as a function of microstructure by means of polycrystal homogenization strategies [1]. These tools are extremely valuable for microstructural design towards more efficient and safe used of materials.

Finally, and especially in the case of nanostructured materials, knowledge on the deformation mechanisms responsible for their high strength is still lacking, and in situ nanomechanical testing is crucial to identify these novel mechanisms. Figure 3 shows an example for an Al/SiC metal-ceramic nanolaminates. The in situ studies in the TEM allowed to conclude that dislocations were emitted and annihilated at the interfaces during deformation in the case of nanometer thick Al layers. The need to continuously nucleate dislocations at the interfaces explains the high strength of these nanocomposite

Figure 2. (a) Micropillars machined by FIB on the surface of a wrought Inconel 718 alloy. (b) Deformed pillar on the <012> orientation showing the activation of different slip systems. (c) In-situ micromechanical stage to carry out tests in the SEM at temperatures up to 800°C.

Figure 3. (a) In-situ nanomechanical stage to carry out tests in the TEM. (b) Image of an Al/SiC nanolaminate being compressed inside a TEM.
materials and this information could only be determined from *in situ* experiments, as *post-mortem* analysis revealed dislocation free nanostructures even in the case of heavily deformed nanolaminates.

**Dual scale determination of damage mechanisms in fiber-reinforced polymers by XCT**

Deformation mechanisms and damage development in fiber reinforced composite materials is a complex process that involves several damage mechanisms that interact together during failure. The complexity of failure mechanisms leads to anisotropy and heterogeneous damage distribution in the laminates. For instance, Figure 4b shows the inhomogeneous damage distribution in a $[\pm 45]_{2s}$ carbon fiber reinforced polymer laminate tested in tension. Short cracks generate at the laminate edges and propagate towards the interior of the laminate leading to a large crack density concentration at the edges. The matrix cracking density is also heterogeneous through the laminate thickness and depends on the interaction with other damage mechanisms [2].

![Diagram](image)

*Figure 4. (a) Set-up of in-situ tensile device at a synchrotron beamline (b) 3D reconstruction of the tomographic volumes of a sample after deformation. Damage by matrix cracking is shown in red and the composite material in semitransparent. (c) Details of damage propagation mechanism ahead of a crack and matrix cracking at a $\pm 45$ interface with toughening particles. (d) 3D reconstruction of a sub-volume at a $\pm 45^\circ$ ply interface. Cracks at $+45^\circ$ and $-45^\circ$ from the interface are shown in red as well as the damage within the interface. The toughening particles at the interface are shown in semitransparent gray color.*
A closer look at one of the crack tips from in-situ synchrotron tomography data (Figure 4c), revealed that the crack propagates within the ply by the formation of micro-porosity which will eventually lead to cusp formation and finally to further crack propagation. The interface of this particular material was reinforced with toughening particles and the damage was in the form of decohesion between particles and matrix. These particles had an important role in delaying the crack propagation and delamination at the interface. The type of damage resembled the cusp formation but cracks rotate when passing through the interface surrounding the particles. This was made visible in the 3D representation of the damage at the interface (Figure 4d), together with cracks at +45° and -45° at both sides of the interface and the toughening particles.

**In-situ XCT infiltration of fibers by vacuum assisted resin transfer molding process**

Fiber-reinforced polymers are extensively used in the automotive, aerospace and energy industries for structural applications. The interest in Liquid Composite Molding (LCM) processes, for the production of composite materials has grown in the last years, especially

![Image of infiltration device and fiber tow showing trapped voids and flow front meniscus.](image)

**Figure 5:** Set-up of the infiltration device. a) Longitudinal cross section of the impregnated tow showing trapped voids and the flow front meniscus. Local fiber misalignments with convergent/ divergent trajectories are also visible. (b) 3D rendering of fiber two showing dry and impregnated regions.
in the vacuum assisted resin transfer molding (VARTM) process due to its relative low cost and the possibility to process large panels, such as wind turbine blades. However, the large amount of physical variables that control the infusion process impacts on the quality of the panels and the physical process is not well understood. Therefore, an in situ infiltration device was developed at IMDEA Materials Institute (Figure 5) to investigate the infusion process by XCT. It was found that the liquid flow in the panel exhibited a dual scale behavior in which the fiber tows saturated at a much slower rate (microflow) than the bulk preform, i.e. between the tows (macroflow) (Figure 5b). Figure 5a shows voids that are formed as a result of the differences in the longitudinal flow within the tows. The migration of the voids along the tow was sometimes constrained by the presence of two fibers with convergent trajectories that could trap the void and arrest the propagation, limiting the microflow. The resin flow process through the fiber fabric is therefore very complex and understanding the parameters that control the nucleation, growth and coalescence of voids during infusion using XCT is key to improve the VARTM process. Details of this research can be found in [3].

References


Functional intercalation in LDH: Towards high performance polymer nanocomposites

Nanotechnology provides a new strategy to develop flame-retardant polymer materials. Compared to conventional flame retardants, the incorporation of nano-additives leads to impressive effects on the heat release rate during combustion of polymers. For instance, the incorporation of 10 wt% of clay into polypropylene led to as much as a 70% decrease in the peak of heat release rate (pHRR) observed in the cone calorimeter test [1]. Besides the improvement in flame retardancy, the addition of nano-additives can increase the mechanical properties as well, whereas most of the conventional flame retardants lead to the opposite effect. Among various nano-additives, layered double hydroxide (LDH), as a typical inorganic layered crystalline material, has aroused much interest in the field of polymer nanocomposites [2]. LDH has been proven to be a very efficient additive to improve the mechanical properties, thermal stability and flame retardant performance of polymers [3, 4]. However, the homogeneous dispersion of LDH into the polymer is a critical factor to achieve the optimum performance.

In order to obtain a homogeneous dispersion and optimized properties, the High Performance Polymer Nanocomposites Group of IMDEA Materials Institute has developed a series of novel functionally-intercalated layered double hydroxides. A good example is the synthesis of multifunctional LDH intercalated by hydroxypropyl-sulfobutyl-beta-cyclodextrin (sCD), phytic acid (Ph), sodium dodecylbenzenesulfonate (SDBS) and chalcone (Figure 1). These compounds are introduced to modify the properties. For instance, hydroxypropyl-sulfobutyl-beta-cyclodextrin (sCD) and phytic acid (Ph) enhance the flame retardancy, whereas sodium dodecylbenzenesulfonate (SDBS) increases the interlayer spacing and chalcone provides better resistance to ultraviolet radiation.

As compared with the pure epoxy and the unmodified LDH/epoxy, the pHRR of multifunctionalized LDH/epoxy nanocomposite was dramatically reduced to 232 kW/m², a 72% reduction compared to that of pure epoxy (Figure 2). Besides the improvement of flame retardancy, the addition of the multi-intercalated LDH also led to an excellent resistance to ultraviolet radiation. Optical micrographs in Figure 3 show the specimens before and after being subjected to the ultraviolet radiation for 400 hours. Surface micro-cracks were found in pure epoxy and unmodified LDH/epoxy after ultraviolet irradiation, while no significant changes were detected in the morphology of the multi-functionalized LDH/epoxy nanocomposite.
In another study, the effect of the char residues on the flame retardant mechanisms were ascertained in unmodified LDH/epoxy and functionalized LDH/epoxy nanocomposites, Figure 4 [5]. The quality of the char residue correlates with the homogeneous dispersion of the nanofiller in the polymer matrix. The unmodified LDH is apt to form aggregated stacks in the epoxy matrix, and thus, the residue shows a cracked surface without sufficient cohesion. In contrast, the well-dispersed functionalized LDH leads to a compact and continuous residue, which can serve as an excellent insulator and a mass transport barrier, simultaneously, leading to an improved fire retardancy.

References

Computational and data-driven materials discovery

New materials play a key role in meeting the challenges of many emerging technologies in energy, healthcare, security and structural applications. Computation has played a pivotal role in understanding the molecular or material design process and in boosting the discovery of novel and useful chemical systems. Indeed, molecular simulation techniques have advanced to the point that accurate “forward” predictions can be made to determine the properties and performance of a given chemical system. The push for additional computational power has been mainly focused on building and improving these simulation tools, including more accurate methods and/or enabling studies of larger systems via multiscale approaches.

However, a materials designer often has a specific property in mind, such as the emission/absorption wavelength, the particular band structure, or the adsorption selectivity for gas mixtures. The goal of this “inverse problem” is to search for stable materials that display the desirable value of the targeted property. Solving this inverse problem by exhaustively searching for a chemical system with the requested property or performance is impractical: the number of systems that can be synthesized is often so large that only a small fraction of all possible structures can be addressed by brute force screening. Instead, the IMDEA Materials’ Computational and Data-Driven Materials Discovery group has been developing strategies and approaches that enable identification of the best molecule or material for a given application at a minimal computational cost.

The group develops and employs a hybrid material informatics-molecular simulation approach to materials discovery. This approach involves: (i) exploration of the material space by curating large databases of experimental structures as well as enumeration of novel, yet-to-be-made materials, (ii) material informatics methodology involving custom descriptors and similarity measures, (iii) machine learning and optimization-based approaches to selected structures that undergo extensive characterization using molecular simulations.

The hybrid discovery approach employing (i)-(iii) can be adapted to various classes of materials and applications. So far it has been used to discover materials for gas separations and storage [1-3]. Figure 1 highlights how (i)-(iii) was used to map one property, i.e. density, in a set of 183 090 predicted ionic liquids (IL) materials while computationally character-
izing less than 30 systems. The latter represented the statistically-relevant diverse set, and were used to build a machine learning model correlating the structure with the property (density is illustrated in Fig. 1, for other properties see [1]). The machine learning-based predictions were later confirmed for a set of randomly selected ILs, see Fig. 1.

References


Figure 1. (top) Map of chemical space of 183 090 ionic liquids (IL) with triazolium-based cations and the bis(trifluoromethanesulfonyl)-amide (Tf₂N⁻) anion. Blue dots correspond to the diverse ILs, which were characterized using molecular simulation, and then used to build a neural network model correlating the structure with simulated property. Red dots, marked E1–E14, are representative structures which underwent synthesis and characterization. Horizontal and vertical axes correspond to the largest principal components in the cation descriptor space. (bottom, left) Neural network model prediction of density for all considered ILs. (bottom, right) Experimental verification of the approach for randomly selected IL.
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