foreword

Javier LLorca
Director, IMDEA Materials Institute
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annual report 2016
Materials Science and Engineering has been at the root of new technological developments because they are always supported by a material substrate. Thus, materials research is sometimes driven by applications and sometimes by the materials themselves. In the latter case, research lines run parallel to the different families of materials: metals, polymers, ceramics and, more recently, biomaterials, composites as well as nanomaterials. During the first ten years, IMDEA Materials Institute has developed an expertise in the processing, characterisation and modelling of these types of materials, which was then applied –in collaboration with our industrial partners– to different sectors in the areas of transport, information technology and manufacturing, as well as in the exploration of emerging materials and processes for sustainable development. However, the Institute is aware of the societal challenges that lay ahead in the fields of energy and health care and has decided to attract expertise in these two fields in the following years. Two new research lines were opened during 2016 in electrochemistry and in solar energy harvesting and luminescence to widen the activities of IMDEA Materials Institute in energy. Together with the current activities in the development of structural materials for energy harvesting and storage –supported by the European Research Council–, IMDEA Materials is now ready to develop new materials designed to support the energy challenges of the society.

While the research output of an academic institution is usually measured by the quality and impact of the publications, patents and industrial applications of the knowledge developed, funding –particularly in competitive calls– is also a measure of success. It provides the means to carry out the research and indicates the capability of the Institute to articulate credible research goals that go beyond the state of the art. Since the beginning of its activities in 2007, IMDEA Materials Institute has been able to attract over 26 millions of euros from external funding sources. 50% of the funding was obtained from competitive calls of the European Union while 23% came from research contracts with industrial companies. In particular, IMDEA Materials Institute has been very successful in the highly competitive calls of the pillar of excellence (European Research Council, Marie-Slodowska Curie actions, etc.) of the Horizon 2020 program with 5.7 million euros in research grants during the period 2014-2016.

The outcome of the research activities performed during 2016 is summarized in the following pages. The personnel, current research projects, research infrastructures as well as disseminations activities (publications, conferences and seminars, patents, theses, etc.) can be found in this annual report together with a few scientific highlights on advanced materials for multifunctional applications, additive manufacturing, and the development of an open source library of material models.
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1. Introduction

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1.1. About IMDEA Materials Institute

The IMDEA Materials Institute (Madrid Institute for Advanced Studies of Materials) is a non-profit independent research organization 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, an institutional framework created in 2007 to foster social and economic growth in the region of Madrid by promoting excellence in research 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.

IMDEA Materials Institute has built an international reputation in the areas of design, processing, characterisation and modelling of advanced materials for applications in different industrial sectors with particular emphasis in transport, energy and manufacturing. The core strength of the Institute is its international research team, consisting of talented researchers from 14 different nationalities, that carry out new scientific discoveries in materials science, and foster the development of emerging technologies.

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. This combination provides the institute the ability to address technological challenges in collaboration with companies to create value in their products and processes through novel knowledge that will be transformed into technological innovations.
1.2. Organizational chart

Figure 1. Organizational chart of IMDEA Materials Institute.

1.3. Appointments to the Board of Trustees and Scientific Council

Prof. Manuel Doblaré, Scientific Director, has resigned as trustee in representation of Abengoa Research S.L.

Prof. Andrew I. Cooper, Director of the Materials Innovation Factory, University of Liverpool, 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.
1.4. Governing bodies

1.4.1. 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
Coordinator of the Area of Research, 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
Professor University of Karlsruhe, Germany

Prof. Andreas Mortensen
Vice-provost for Research Professor
Ecole Federale Polytechnique of Lausanne, Switzerland

Prof. Trevor William Clyne
Professor
Cambridge University, UK

Prof. Dierk 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.
Seville, Spain

GRUPO ANTOLIN S.A.
Mr. Javier Villacampa, Corporate Innovation Director
Burgos, Spain

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

SECRETARY

Mr. Alejandro Blázquez
1.4.2. 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. Dr. Andrew I. Cooper
Director, Materials Innovation Factory
Professor
University of Liverpool, UK

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

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. Andreas Mortensen
Vice-provost for Research
Professor
École Fédérale 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. Juan Manuel Rojo
Emmeritus Professor
Complutense University of Madrid, Spain

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 in five research programmes devoted to:

- Advanced materials 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 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 2. Research programmes and strategic partners of IMDEA Materials Institute
Advanced Materials for Multifunctional Applications

The Programme on Advanced Materials for Multifunctional Applications at IMDEA Materials Institute combines expertise in design and synthesis of nano and molecular building blocks and their integration into macroscopic materials and devices. The guiding objective is to simultaneously realise various functions, including fire safety, high-performance mechanical properties and efficient energy management, amongst other properties. 34 researchers in the programme combine expertise spanning from in silico molecular design to fabrication of large energy storing devices. The following are the main research lines of the programme:

- **Synthesis, emerging technologies and integration of carbon-based nanomaterials (graphene, nanotubes, nanofibres and hybrids):**
  - Nanomaterials integration towards devices and energy managing devices: synthesis of nanocarbon/semiconductor hybrids for photo and electrocatalysis, interaction of nanocarbons with liquid molecules, polyelectrolytes and inorganic salts.
  - Sensors: chemical, piezoresistive, piezoelectric.
  - Hierarchical materials: materials design from the nanoscale to the macroscale, nano-reinforced materials, composite materials with enhanced electrical and thermal conductivity.
  - Size effects in the mechanical behaviour of multifunctional materials: study of structure-property relations in macroscopic ensembles of nanobuilding blocks, and development of mechanical models for hierarchical materials and their interfaces.

- **Synthesis and properties of polymer-based multifunctional nanocomposites:**
  - Sustainable materials: bio-based nanocarriers, novel guest-host nanomaterials, nano-cross linkers, functional dye-sensitized solar cells, multifunctional polymer nanocomposites, etc.
  - Fire retardant materials through nanodesign: multifunctional nanomaterials to increase fire retardancy: layered double hydroxides, sepiolite, molybdenum disulphide (MoS₂), nanocarbon, nano metal hydroxide, novel functional nanomaterials, nanocoatings, etc.

- **Computational and data-driven Materials Discovery**
  - Discovery of porous materials for energy applications (CO₂ capture, methane storage).
  - Design of ionic liquids.
  - Characterisation of nanoparticles and others.
• Electrochemical Energy storage
  
  - Tailored designing of nanostructured electrode materials, interfaces and electrolyte compositions.
  - Spectroscopic/microscopic studies and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O$_2$.

Link to relevant research projects

Research groups involved:

- **Multifunctional Nanocomposites**
  Dr. J. J. Vilatela
  *Programme leader*

- **High Performance Polymer Nanocomposites**
  Dr. D.-Y. Wang

- **Computational and Data-Driven Materials Discovery**
  Dr. M. Haranczyk

- **Electrochemical Energy Storage, Nanomaterials**
  Dr. V. Etacheri

- **Nano-architectures and Materials Design**
  Dr. R. Guzmán de Villoria
The Next Generation of Composite Materials

The Next Generation of Composite Materials Programme aims at developing solutions for high performance structural composites with enhanced multifunctional capabilities such as thermal, electrical and fire resistance. The programme is focused on key aspects of material science and engineering including manufacturing, optimisation of material performance (damage tolerance and impact resistance), material characterisation at different length scales (nanoindentation, X-ray tomography) and development of modelling tools for both virtual processing and virtual testing. Manufacturing of composites by injection/infusion/pultrusion or prepreg consolidation is assisted by advanced sensors that support the use of smart manufacturing techniques toward process optimisation. Multiscale physically-based simulation tools are envisaged to predict the mechanical performance of structural composites as a function of their structure allowing a significant reduction of costly experimental campaigns. The main research lines of the programme are shown below.

- **Processing of high performance composites:**
  - Optimisation of out-of-autoclave processing (injection/infusion/pultrusion or prepreg consolidation) and other manufacturing strategies (semicured products). Hot-forming. Non-conventional curing strategies.
  - Smart manufacturing processes based on advanced simulations and sensors.

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

- **New frontiers of structural performance:**

- **Composites with multifunctional capabilities:**
- **Micromechanics of composites:**
  - In situ measurement of matrix, fibre and interface properties. Micromechanical-based failure criteria. Computational-design of composites with optimised properties (non circular fibres, thin plies, novel fibre architectures, etc.)

- **Virtual testing of composites:**
  - Multiscale strategies for design and optimisation 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:**

**Research groups involved:**

- **Structural Composites**
  - Dr. C. González
  - Programme leader

- **Design & Simulation of Composite Structures**
  - Dr. C. López

- **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

The programme, integrated by experts in physical simulation, solidification and casting, physical metallurgy, solid state processing and computational materials engineering, aims to explore the processing-structure-property relationships in bulk metals, with special emphasis on the role of microstructure on plasticity at all length scales. This interdisciplinary pool of researchers is formed by physicists, chemists, and engineers (materials, mechanical and aeronautical) carrying out fundamental research and also working in close collaboration with companies in the transport, aerospace, energy and biomedical sectors. Research facilities include state-of-the-art equipment for processing at a lab scale (casting, wrought processing, Gleeble technology, atomization), microstructural characterisation (electron microscopy, X-ray diffraction, nanotomography) and mechanical property testing at a wide range of temperatures and strain rates. The main research lines of the programme are listed below.

- **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. Mg alloys and nanocomposites for green transport.

- **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.

- **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.
  - Design of metallic powders for additive manufacturing.
• **Solidification and Casting:**
  - Optimisation 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).

• **Physical simulation of metallurgical processes:**
  - Development of novel thermo-mechanical processing routes for the fabrication of metallic materials with superior properties. Design and optimisation 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 mechanical properties.

Link to relevant research projects

**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
• **Model-based materials design:**

  - Integration of modelling tools (atomistic, computational thermodynamics and kinetics, phase field) to simulate the microstructural development of materials during processing.

• **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 of structural components.

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**Integrated Computational Materials Engineering**

The research program on Integrated Computational Materials Engineering (ICME) is aimed at integrating all the available simulation tools into multiscale modelling strategies capable of simulating processing, microstructure, properties and performance of engineering materials, so new materials can be designed, tested and optimized before they are actually manufactured in the laboratory. The focus of the program is on materials engineering, i.e. understanding how the microstructure of materials develops during processing (virtual processing), the relationship between microstructure and properties (virtual testing) and how to optimize materials for a given application (virtual design). Moreover, experiments are also an integral part of the research program for the calibration and validation of the models at different length and time scales.

The expertise of the researchers in the program covers a wide range of simulation techniques at different scales (electronic, atomistic, mesoscopic and continuum) and is supported by a high performance computer cluster.

The following are the main ICME research lines at IMDEA Materials Institute.

• **Virtual materials design, including virtual processing and virtual testing:**

  - Light (Al, Mg and Ti) metallic alloys and their composites. Ni-based superalloys. Multifunctional composite materials and structures. Materials for energy generation and storage.
• **Materials modelling at different length and time scales:**
  

• **Multiscale materials modelling:**
  

**Link to relevant research projects**

**Research groups involved:**

- **Design & Simulation of Composite Structures**
  
  Dr. C. López  
  *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. M.j Haranczyk
Multiscale Characterisation of Materials and Processes

Progress in the development of new materials and processing methods can only come from a thorough understanding of microstructure evolution, either during processing or during service operation. Since the microstructural features that determine the material behaviour usually span several length scales (for instance, from the macroscopic defect distribution to the nanometer scale precipitates in the case of metallic alloys), this understanding can only come from advanced 4D characterisation techniques, capable of determining the evolution of the 3-dimensional microstructure over time at different length scales (hence the name 4D). This is precisely the objective of this programme, i.e., to understand microstructure/defect evolution in advanced materials during processing and service using advanced characterisation techniques, such as:

- **3D Characterisation of materials**, including microstructural, chemical and crystallographic information across several scales:
  - X-ray tomography and diffraction.
  - Scanning electron microscopy and focus ion beam, including 3D energy-dispersive X-ray microanalysis and electron back-scatter diffraction.
  - Transmission electron microscopy, including 3D energy-dispersive X-ray microanalysis and tomography.
  - Multiscale correlative tomography studies, i.e. tomography across multiple scales by 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, etc in the scanning electron microscope and X-ray tomography scanner. Properties and deformation mechanisms of small volumes by nanomechanical testing in the scanning and transmission electron microscopes: properties of metallic phases, interfaces, nanoparticles, carbon based nanomaterials (carbon nanotubes, graphene, ...).
  
  - Elevated temperature nanomechanical testing.
  

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

**Link to relevant research projects**

**Research groups involved:**

- Nanomechanics  
  Dr. J. M. Molina-Aldareguía  
  *Programme Leader*

- X-Ray Characterization of Materials  
  Dr. F. Sket

- Multifunctional Nanocomposites  
  Dr. J. J. Vilatela

- 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

3.1. Senior Researchers [24]
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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 consists of 16 staff researchers, 3 visiting researchers, 29 post-doctoral researchers and 59 doctoral students from 14 different nationalities plus approximately 20 master students. It should be noted that 40% of the researchers are foreign nationals while 50% 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 eight 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 in 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; analysis of the relationship between microstructure and mechanical properties in advanced structural materials.

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**Prof. Ignacio Romero**
Deputy Director, Computational Solid Mechanics
Ph. D. in Civil Engineering, from University of California Berkeley, USA
Professor of Mechanics, 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
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 as 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. 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. 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 nanindentation and advanced focus-ion beam and electron microscopy analysis, mechanical testing inside the scanning and transmission electron microscopes.

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; and 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  
His group’s work is largely focused on the development of macroscopic materials made up of nanobuilding blocks in a way that the unique properties at the nanoscale are preserved through the assembly process and a new generation of high-performance engineering materials is produced. Central to this work is a process to make continuous macroscopic fibres made up of CNTs. The group works actively in studying their hierarchical structures by advanced X-ray techniques, reinforcement at multiple length-scales and the electrochemical interactions of CNT fibres with liquids and polymers. This research has helped establish the unique combination of properties of CNT fibres, and is enabling the fabrication of multifunctional composites that can store energy or have sensing functions.
Dr. De-Yi Wang  
Senior Researcher, High Performance Nanocomposites

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

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

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.
researchers

Dr. Vinodkumar Etacheri  
(New incorporation)  
Researcher, Electrochemical  
Energy Storage,  
Nanomaterials  
Ph.D. in Materials Chemistry from  
Dublin Institute of Technology,  
Ireland  
Research Interests  
Tailored designing of nanostructured electrode materials, interfaces and electrolyte compositions, their spectroscopic/microscopic study and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O₂ batteries.

Dr. Roberto Guzmán de Villoria  
Researcher, Nano-Architectures and Materials Design  
Ph.D. in Mechanical Engineering from the University of Zaragoza, Spain  
Research Interests  
Nan-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  
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 fibre-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; and incorporation of experimental results to the development of physically-based models for optimisation of material processing and properties.
visiting scientists

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. Development of mechanical metamaterials using elastic instabilities; hybrid nano- and micro-structured material systems; multiscale modelling and simulation; design optimisation 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.

Prof. Shibin Nie
Visiting Scientist, Bio-based fire retardant materials
Ph.D. in Polymeric Chemistry from University of Science and Technology, China
Associate Professor, Energy Resources and Safety, Anhui University of Science and Technology, China
Research Interests
Thermal and flame retardant properties of polymer nanocomposites; synergistic effect of metal compounds with intumescent flame retardants, such as metals, metal oxides, metal salts, metal chelates; catalyzing carbonization of polymer nanocomposites; thermal and flame retardant properties of semibioocomposites or bio-composites based on starch and lignin.

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; strength and fracture response of materials 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; and advanced finite element simulations combined with crystal plasticity and nonlocal damage models to predict the deformation and fracture of complex materials.
Dr. Belén Aleman  
Postdoctoral Research Associate  
Ph.D. in Physics from Complutense University of Madrid, Spain  

Research Interests  
Synthesis of continuous macroscopic fibres made up with carbon nanotubes with molecular control to fix the final macroscopic properties of the material; chemical and structural analysis by X-ray synchrotron radiation based diffraction and XPS microscopy; and vacuum systems development for gas phase simulation experiments under UV radiation and plasma.

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; 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; and 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. Marco Bernabei  
Postdoctoral Research Associate  
Ph.D. in Physics from University of the Basque Country University, Spain  

Research Interests  
Atomistic modelling and computer simulation techniques for the design and characterisation of new porous materials in crystalline and/or amorphous solid state.
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; optimisation of the production method to obtain a highly pure material; modification of nanostructure properties after purification treatments; and 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  
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. Daniel Cintora  
Postdoctoral Research Associate  
Ph.D. in Materials and Energy from University of Córdoba, Spain  

Research Interests  
Synthesis, characterisation and application of materials for energy storage and conversion; electrochemistry of inorganic materials, conducting polymers, polymer electrolytes, hybrid materials, composite electrodes, and their application in devices such as batteries and fuel cells.

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. Soundes Djaziri  
Postdoctoral Research Associate  
Ph.D. in Materials Physics from University of Poitiers. France  

Research Interests  
Structure-property connections for functional materials; crystal structure characterisation and stress measurements using X-ray diffraction methods (laboratory and synchrotron sources); In-situ studies under extreme environments (physical or thermo-mechanical) of composite materials by X-ray diffraction, radiography or electron microscopy.

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

Research Interests  
Design of advanced composites laminates with non-conventional architectures manufactured by means of advanced fibre placement; numerical analysis and simulation of progressive damage and failure in variable stiffness composite panels experimental studies of “low-drop” defects under in-plane and impact loading; and damage resistance and damage tolerance analysis in variable stiffness composite panels.

Dr. Juan Pedro Fernández  
Postdoctoral Research Associate  
Ph.D. in Chemistry from the Complutense University of Madrid. Spain  

Research Interests  
Processing and characterisation of polymer-based nanocomposites; study of the effect of the nano-compounds 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, optimisation of the mechanical properties of metallic alloys by modification of their processing route; optimisation of novel structural materials for energy generation plants; and fabrication of oxide-dispersion strengthened alloys by powder metallurgy and optimisation 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 optimisation.

Dr. Sandip Haldar  
Postdoctoral Research Associate  
Ph.D. in Mechanics and Materials at the University of Maryland, College Park. USA  
Research Interests  
Solid mechanics; composite materials; and experimental mechanics.

Dr. Sarra Haouala  
Postdoctoral Research Associate  
Ph.D. in Engineering Sciences at the Université Catholique de Louvain. Belgium  
Research Interests  
Computational mechanics of materials; and multi-scale modelling of heterogeneous materials.

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; and environmentally friendly thermoset polymers from renewable feedbacks.
Dr. Anna Hynowska  
Postdoctoral Research Associate  
Ph.D. in Materials Science from Autonomous University of Madrid. Spain  
Research Interests  
Complex shaped Fe-Al intermetallic parts development by reactive infiltration method.

Dr. Hong Liu  
Postdoctoral Research Associate  
Ph.D. in Materials Science and Engineering from University of Monash. Australia  
Research Interests  
Study of microstructure evolution and deformation mechanisms of light alloys (e.g. Mg and Al based alloys) and their microstructural characterisation by means of phase field method.

Dr. Amitava Moitra  
Postdoctoral Research Associate  
Ph.D. in Engineering (Applied) Physics from Mississippi State University. USA  
Research Interests  
Integrated computational materials engineering; density functional theory; large scale atomistic simulations, molecular dynamics, semiempirical potential generation (EAM/MEAM); and deformation mechanisms in HCP materials.

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. Joseba Múgica  
Postdoctoral Research Associate  
Ph.D. in Mechanics and Manufacturing from Mondragón University. Spain  
Research Interests  
Characterisation of the mechanical behaviour of composite materials and fibre metal laminates; computational micro and mesomechanics of composite materials; and impact and damage tolerance analysis of composite structures.

Dr. David Portillo  
Visiting Postdoctoral Research Associate  
Ph.D. in Nuclear Fusion from Polytechnic University of Madrid. Spain  
Research Interests  
Numerical methods for solid and fluid mechanics; simulation of laboratory plasma physics experiments; and inertial confinement fusion.
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 nonstoichiometric silicon oxide films; thermodynamics and kinetics of metal induced crystallisation of amorphous and disordered Si; and 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; and 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; and UV-curing flame retardant coatings.

Dr. Xin Wen  
Postdoctoral Research Associate  
Ph.D. in Chemistry and Physics of Polymers at Changchun Institute of Applied Chemistry, China.  
Research Interests  
Synthesis and application of carbon materials; and high-performance (nano) composites of polymers

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Postdoctoral Research Associate  
Ph.D. in Computational Science in Engineering from University of Leuven, Belgium  
Research Interests  
Quasi-static and fatigue damage modelling/experiment; multiscale modelling impact and damage tolerance analysis of composite structures.
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Research: Modelling of ice impact on jet turbines

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Research: Kinetics of Magnesium Alloys

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Research: Nano-architectures and materials design

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Research: Nanoindentation of light alloys

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Research: Solidification processing and properties of Zn-Al hypoeutectic alloys

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Research: High strain rate mechanical behaviour of advanced high strength steels

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Research: Dislocation dynamics simulations of strengthening in metallic alloys

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Research: Nanostructured supercapacitors
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Research: Computational Thermo-dynamics of Magnesium Alloys

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Research: High throughput diffusion and phase transformation

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

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Research: Voids in out-of-autoclave prepregs

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Research: High-strength steels

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Research: Multifunctional nano-materials based polymer nano-composites

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Research: Polymer composites and nanocomposites

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Research: Polymer nanocomposites
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4.1. Synthesis, processing and integration of materials [46]
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4.1. Synthesis, processing and integration of materials

Metallic alloys

- **Arc Melting and Casting Furnace** (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 the 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.

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

- **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).
Polymer based composites and nanocomposites

- **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, Magnus 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.

- **Micro compounder** (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.

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

• **Chemical Synthesys Laboratory** (built in-house, IMDEA Materials Institute) to carry out chemical synthesis, including organic, inorganic and nanomaterial synthesis, aiming at creating and functionalizing new materials.

**Nanomaterials**

• **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 ºC).

• **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.
Batteries

- **Ar-Filled Glove Box** (Vigor Sci-Lab) that can achieve high-purity (99.999%) Ar-atmosphere required for fabricating rechargeable batteries (Li, Na, K-ion, Li/Na-S, Li-O₂ systems). The system is equipped with oxygen and moisture sensors and absorbers. Oxygen and moisture levels less than 1 ppm can be achieved in this glove box system. *(New equipment)*

- **Coin cell battery fabricator** (MTI) to fabricate various types of 2032-type coin batteries for electrochemical testing. This system can be also employed for opening the coin cells after electrochemical testing to perform postcycling microscopic/spectroscopic analysis. *(New equipment)*

- **Hydrothermal System** (Parr Instruments) to synthesis metal oxide and carbon based materials for functional applications including electrochemical energy storage. Temperature can be adjusted upto 300 °C and the total volume of the reactor is 200 mL. *(New equipment)*

- **Tube Furnace** (MTI) to synthesize materials through reduction and oxidation reactions depending up on the working gas selected. Temperatures up to 1200 °C can be achieved in Ar, N₂, Air, NH₃ and H₂ atmospheres. Outlet of the tube furnace is connected to a water trap to remove byproducts produced during the material synthesis. *(New equipment)*

- **Planetary Mixer** (Thinky SR-500) to homogenise the electrochemically active material with conductive carbon additive and binder in a suitable solvent. The slurry obtained can be uniformly coated on Cu or Al foils to prepare electrodes for rechargeable batteries. *(New equipment)*

- **Vacuum Oven** (Thermo Scientific) to remove solvents and drying the electrode materials for rechargeable batteries. A maximum operating temperature of 250 °C and vacuum of 10 mbar can be achieved. *(New equipment)*
4.2. Microstructural and chemical characterisation

- **Field-Emission Transmission Electron Microscope** (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 webpage of the institute (http://materials.imdea.org/research-infrastructure/services-rates/external-use-of-tem/)

- **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.
• **Ram Micro spectroscopy system** (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** (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** (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.
4.3. Mechanical properties

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.

- **Fibre Mechanical Testing Machine** (FAVIMAT+) to characterize fibre mechanical properties, as well as linear density and crimp. Measurement of the mechanical properties in a liquid medium is also possible.

- **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 – 600°C, 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 25°C to 400°C.

**Nanomechanics**

• **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.
4.4. Functional properties

Thermal

- **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.

- **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 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. This DSC equipment is also coupled
with a **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.

- **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.

- **Horizontal Pushrod Dilatomer (New equipment)** (DIL 402 Expedis Supreme, NETZSCH) for the measurement of dimensional changes as a function of temperature on the basis of DIN EN 821, DIN 51045, ASTM E831 or ASTM E288 standards. The measurements can be carried out in vacuum, inert or oxidizing gas atmosphere. The dilatometer is equipped with a novel “NanoEye” optoelectronic sensor with unmatched resolution over the entire measuring range, which allows direct sequential measurement of samples of different lengths and with different expansion behaviour at maximum precision.

### Fire resistance

- **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.

- **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.

**Electrochemical**

- **Battery tester** (Neware BTS 4000, Neware) to perform the evaluation of secondary batteries through galvanostatic charge discharge tests. Each channel can handle 0 to 10 mA current and 0 to ±5V potential. One unit can simultaneously test 8 different batteries and different current densities. Charge-discharge measurements can also be performed at elevated temperature. *(New equipment)*

- **Electrochemical Workstation** (Zive SP1) to perform a wide range of electrochemical tests (Including galvanostatic, potentiostatic and electrochemical impedance spectroscopy) for characterizing batteries, supercapacitors as well as corrosion protection coatings. Current and voltage ranges are 1A and 10 V, respectively. Built in frequency generator can produce AC waves of up to 1MHz frequency. *(New equipment)*
• **Karl Fischer Moisture Analyser** (TOB Energy) to measure moisture content in various solvents up to 1 ppm level. This ensures the preparation of moisture free electrolytes for rechargeable batteries. *(New equipment)*

• **Conductivity Meter** (TOB Energy) to measure the ionic conductivity of electrolyte solutions. The equipment is capable of temperature compensation (-20 to 100 °C) during the conductivity measurement. *(New equipment)*

• **Two-channel Potentiostat** (ECLab SP200, BioLogic) with EIS and nano-current modules to carry out electrochemical studies. *(New equipment)*

**Electrical and optical**

• **Source-meter unit** (2450 Keithley) for electrical characterisation of devices and measurement of nanocurrents. *(New equipment)*

• **150W Xe lamp** (67001, Newport) and **Electrochemical Cell** for photoelectrocatalytic studies. *(New equipment)*

• **Microprobe Station** for electrical characterisation of optoelectronic devices. *(New equipment)*

**4.5. Simulation**

**High performance computing**

• High Performance Computer cluster with 600+ Intel Xeon CPU cores and NVIDIA GPU acceleration leading to a computational power of 90 Tflops

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

• Commercial and open source software tools for modelling and simulation in Materials Science and Engineering (CALPHAD, DICTRA, Micress, Abaqus, LS-Dyna, PamCrash, LAMMPS, etc.).
Simulation tools

**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 optimisation 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 (VIrtual Ply propERty) is a simulation tool developed within the framework of computational micromechanics by IMDEA Materials to predict ply properties of fibre-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 optimisation.

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

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, please visit: http://materials.imdea.org/research/simulation-tools/
Current research projects 5

Annual report 2016
The Institute has participated in 65 research projects in 2016. 14 of these projects started during the year. Although the number of projects has decreased as compared to 2015, the total project funding in 2016 was 23% higher than in 2015. In particular, project funding coming from European and national/regional competitive calls increased by 39% and 66%, respectively, compared to year 2015, whereas funding coming from industrial contracts decreased by 15% year-on-year.

The project portfolio is divided into three main groups: 32 projects were obtained in international competitive calls, out of which 20 were funded by the European Union and 12 by the Chinese Scholarship Council. In addition, 13 projects were supported by research programmes sponsored by the Spanish Ministry of Economy, Industry and Competitiveness and two by the Regional Government of Madrid, while 18 projects were directly funded through industrial contracts. Several of these industrial contracts are supported by the Spanish Centre for the Development of Industrial Technology (CDTI).

![Figure 3. Number of active research projects per year by funding source](image-url)
A brief description of the projects started in 2016 is provided below:

**STEM**

“Structural energy harvesting composite materials”

**Funding:** European Research Council, Starting Grant, European Union-Horizon 2020 Programme

**Duration:** 2016-2021

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

The purpose of this project is the development of new multifunctional structural composite materials that combine high performance mechanical properties and the possibility to harvest energy. The multifunctional composites are based on a continuous macroscopic fibre made up of highly aligned carbon nanotubes that has bulk mechanical, electrical and thermal properties already similar to carbon fibre and the mesoporosity and chemical resistance of an activated carbon; which will be combined with nanostructured semiconductors that can transfer charge/energy when subjected to external stimuli and integrated in a polymer matrix to form composite structures. The project comprises a detailed multiscale study of materials synthesis and properties, including in-situ spec-
DYNACOMP
“Dynamic behaviour of composite materials for next generation aeroengines”

Funding: Marie Skłodowska-Curie-ITN-EID, Horizon 2020 Programme, European Union-Horizon 2020 Programme
Partners: IMDEA Materials Institute (Project Coordinator), HEXCEL, Micro Materials, Technical University of Madrid and Madri+d foundation
Duration: 2016-2020
Principal Investigator: Dr. J. Molina

DYNACOM is an European Industrial Doctorate (EID) programme focused on the design of the next generation of structural composite materials for high strain rate applications. This goal will be achieved by the development of a consistent, physically based multiscale simulation strategy informed by the dynamic properties of the constituents (fibre, matrix and fibre/matrix interface) measured with a novel micromechanical testing.
methodology. The technological focus is put into the introduction of new composite components into the next generation of aeronautical engines, but the implications are numerous in other sectors where composite materials have been identified as a key enabling technology, such as in transport, energy generation and biomedical applications. To accomplish this, the programme brings together one research institution (IMDEA Materials Institute), two industrial partners (HEXCEL and Micro Materials), one academic institution (The Technical University of Madrid) and a non-profit organization (Madri+d).

The joint academic and industrial training programme offered by this EID will ensure that the innovative aspects of the research work find a quick industrial integration and will provide the ESRs with a truly interdisciplinary and intersectoral training, enhancing their employability and career perspectives.

IMDEA Materials Institute coordinates the DYNACOMP project and will lead the scientific direction of the programme.

**ACERCOM**

“Fibre metal laminates for application in marine renewable energy”

**Funding:** Challenges-Collaboration Programme, Spanish Ministry of Economy, Industry and Competitiveness  
**Partners:** ArcelorMittal (Project Coordinator), Technical University of Madrid and IMDEA Materials Institute (Technical Coordinator)  
**Duration:** 2016-2019  
**Principal Investigator:** Dr. C. González

Marine wind energy is playing a key role in the development of renewable energy. The marine wind resource is greater and of better quality than the land one and this makes possible to install more efficient powerful windmills. Moreover, the environmental impact of those off-shore structures is less than the one created by land wind mills. It can be said that generally speaking, marine wind energy has a great potential both at European and Spanish level. However, the installation and maintenance costs of marine windmills has to be reduced in order to allow an increase of the installed power. The development of novel materials is paramount in order to decrease the installation and maintenance costs of marine windmills since they will allow the manufacture of lighter, more efficient designs. Structural steel has traditionally been the material employed for building windmill towers. However, steel has a series of drawbacks (those associated to its weight, fatigue behaviour and corrosion resistance). The weight reduction in windmill towers
will be achieved by the partial substitution of steel by a lighter, more resistance composite material. These materials are manufactured by intercalating sheets of steel and composites, which are known as fibre metal laminates.

The ACERCOM project will incorporate all the structural and functional requirements needed for the design of a novel fibre metal laminate valid for application in marine renewable energy. The ACERCOM project will analyse valid combinations of composite materials and their manufacturing routes via infusion or via pre-impregnated composites. Those materials will be fully characterized with regards to their mechanical properties, resistance to extreme environments and fire behaviour. The conditions for industrial upscaling (machining, joining, conformability, ...) will be also analysed within the project. Within the framework of this ambitious collaborative project, coordinated by ArcelorMittal, IMDEA Materials Institute will mainly carry out the modelling, fabrication and characterisation of fibre metal laminates for application in marine wind energy.

**OPTIQPAP**

“Optimisation of quenched and partitioned steels designed for industrial applications”

**Funding:** Research Fund for Coal and Steel, European Union-Horizon 2020 Programme

**Partners:** IMDEA Materials Institute (project coordinator), Fundació CTM Centre Tecnològic, ThyssenKrupp Steel Europe AG, Universiteit Gent, Centro Sviluppo Materiali, Technische Universität Delft and TATA steel Nederland Technology.

**Duration:** 2016-2019

**Principal Investigator:** Dr. I. Sabirov

Despite significant research on microstructure, strength, ductility and strain hardening of advanced high strength steels processed via Quenching and Partitioning (Q&P) in the current literature, their application related performance has not yet been studied. The OptiQPAP project focuses on the intelligent microstructural design in the high strength Q&P steels for simultaneous improvement of various mechanical properties, which are required for their commercialization. Special attention will be paid to fatigue and fracture behaviour, wear resistance, weldability, ductile-brittle transition temperature, high strain rate behaviour and energy absorption, along with the formability and bendability of Q&P steels.
IMDEA Materials coordinates the OptiQPAP project. The main activities of IMDEA Materials in this project include the analysis of microstructure, fatigue and wear mechanisms, the determination of tensile properties, the study of impact behaviour and the investigation of the low cycle fatigue behaviour. Properties of individual phases will be also analysed.

**EMULATE**

“Multiscale approach for the simulation of thermomechanical problems under severe conditions: application to machining”

**Funding:** National R&D Programme for Societal Challenges, Spanish Ministry of Economy, Industry and Competitiveness

**Partners:** Mondragón University, Technical University of Madrid and IMDEA Materials Institute (Project Coordinator)

**Duration:** 2016-2018

**Principal Investigator:** Prof. I. Romero

Machining of metals is a crucial manufacturing process whose market is estimated to be of the order of 5% of GDP in developed countries. Despite its relevance, the physics of the problem are not well understood and the precise selection of operation parameters has to be tuned by trial and error in many cases (e.g., to ensure the proper tool life or surface integrity conditions in machined components). The next generation of airplane engines, those that can provide increased thrust with reduced environmental impact, require improved machining technologies that can only come from significant advances in the understanding of this process.

EMULATE proposes a multidisciplinary approach to enhance the comprehension of metal machining. For that, three topics will be analysed in order to improve this technology: 1) the development of accurate material models that incorporate the mechanisms of plasticity at the crystal level, as well as the effect of temperature over them; 2) the implementation of robust numerical methods that can upscale the former material models to the macro scale, and remain accurate despite the large deformations in the workpiece; 3) the validation of all material and numerical models with reliable experimental data coming from machining benchmarks, including temperature and microstructure measurements. IMDEA
Materials’ team will be responsible for the formulation, analysis, implementation, and integration of numerical methods for simulation thermomechanical problems. The expected outcomes of the project are of two types: on the one hand, fundamental contributions to material modelling and simulation of thermomechanical processes under severe conditions; on the other, technological improvements in simulation tools and predictive capabilities in machining processes.

**EQUINOX**

“A novel process for manufacturing complex shaped Fe-Al intermetallic parts resistant to extreme environments”

**Funding:** Climate action, environment, resource efficiency and raw materials, European Union-Horizon 2020 Programme

**Partners:** National Technical University of Athens (Project Coordinator), Elastotec GmbH Elastomertechniken, Kochanek Entwicklungsgesellschaft, IMDEA Materials Institute, Technica Univerzita V Liberci, Access e.V., Open Source Management Limited, CES Operations AS, Freni BREMBO Spa, and Yunzhnoye Design Office named after Mikhail Yangel

**Duration:** 2016-2019

**Principal Investigator:** Dr. S. Milenkovic

There is a need to find solutions to replace critical raw materials such as chromium, nickel, molybdenium and vanadium in high volume end consumer products. Steels and superalloys with considerable amounts of these materials are widely used in many industrial applications, particularly under extreme conditions where corrosion and wear resistance are needed. It is generally accepted that intermetallics in particular low cost FeAl offer outstanding material properties. Unfortunately, it is difficult to translate their properties to real products, as intermetallics suffer from low ductility at ambient temperature and poor machinability. The main objective of EQUINOX is to develop a novel process that allows to substitute Cr/Ni based (stainless) steel parts used in high volume end consumer products such as in the lock industry, electronics, process industry...
and automotive industry with a novel near net shape production technology for a new class of highly advanced ductile Fe-Al based intermetallics. Ductility at low to medium temperatures, while maintaining good tensile strength and optimum level of residual stress will be based on a radical new production process that use abundant raw material Fe₃O₄ and Al₂O₃.

IMDEA Materials Institute’s main role in EQUINOX will be to develop a reactive infiltration process with and without the application of pressure. Pressureless infiltration will be performed by drop casting and immersion method. Pressure assisted methods will include suction and centrifugal casting.

**HYDTCOMP**

“Intralaminar hybridization, use of scraps and analysis of their effects. Characterisation and modelling”

**Funding:** National R&D Programme for Societal Challenges, Spanish Ministry of Economy, Industry and Competitiveness

**Partners:** University of Girona (UdG), Project Coordinator and IMDEA Materials Institute

**Duration:** 2016-2018

**Principal Investigators:** Dr. R. Guzmán de Villoria and Dr. C. S. Lopes

Dimensioning transport structures with civil responsibility (e.g. aircraft) accounting for the materials fragility is the main reason to not take full advantage of the excellent elastic properties of carbon fibre composites. Increasing the energy dissipation in fracture events, expand the strain range at which it occurs and, therefore, reduce their brittleness, would directly result in a weight reduction of the component. It is in this context that a stream of research in the international community focused on providing composite materials with pseudo-ductility, through the intelligent use of different concepts of mixture of constituents, which is called hybridization, emerges.

This project concerns the development of technologies for local hybridization in cases where it is necessary (e.g. hybridization during tow spreading). New techniques will be used as the tow spreading, hybrid unidirectional tapes or laminates combining layers of different thickness (thin and traditional thickness) and/or different nature (carbon-glass, carbon-metal). Also a task will be devoted to the use of scraps of automated carbon fibre manufacturing processes to obtain hybrid laminates. The project will include the development of analytical models, advanced simulations (using high performance computing) and microstructural inspection to acquire a physical understanding of the synergistic effects of the hybridization (not yet reached by the
scientific community). Hybrid panels will be manufactured and the mechanical properties experimentally determined. Constitutive models for these materials will be developed as specific tools for design. IMDEA Materials team will develop the techniques of hybridization at (thin) ply level and hybridization by the use of materials scraps at laminate level. Furthermore, IMDEA Materials subproject will play a key role on characterisation and simulation of hybrid composite materials at micro level leading to an insight on the hybridization effects beyond the state of the art.

MATERPLAT

“Advanced materials and nanomaterials spanish technological Platform”

Funding: Technological Platforms Programme, Spanish Ministry of Economy, Industry and Competitiveness
Duration: 2016-2018
Project Coordinator: M. A. Rodiel

Driven by the Spanish Ministry of Economy, Industry and Competitiveness, Technological Platforms are public-private team-work structures led by the industry, in which all the stakeholders of the Science-Technology-Innovation Spanish system interested in a given technological field, work together in a coordinated fashion in order to identify and prioritize medium and long term technological, research and innovation needs. Their main goal is the consecution of the scientific and technological advances that ensure the competitiveness, sustainability and growth of our business network, aligning the strategies of the different stakeholders and focusing R&D&I efforts.

The IMDEA Materials Institute is currently the coordinator, holding the Technical Secretariat since the end of 2016, of the Advanced Materials and Nanomaterials Spanish Technological Platform (MATERPLAT). The platform MATERPLAT, is currently presided by AIRBUS and counts on 170 Spanish associated entities, of which 42% are companies, interested in fostering research, development and the application of Advanced Materials and Nanomaterials. The Management Board of the Platform is formed by AIRBUS, ArcelorMittal, Repsol, B/S/H/, Keraben, CEINNMAT, Regemat3D, Aernnova, Acciona, ITP, AMES, AIMPLAS, Ciber-bbn, Ciemat, ITC, Tecnalia, Sernauto, PTE HPC, MEIC, CDTI and of course, the IMDEA Materials Institute.
NANOFIRE
“Nanomaterials via host-guest interaction as multifunctional fire retardants to polymers”

Funding: China Scholarship Council
Duration: 2016-2020
Principal Researchers: Dr. D. Y. Wang

The project deals with the development of new generation nanomaterials via host-guest interaction as multifunctional fire retardants for polymers. The aim of this work is not only to improve the flame retardancy and mechanical properties of conventional polymers, but also to transfer properties to the polymers, such as UV resistance, thermal conductivity, etc.

MULTICOMP
“Multi-Functional Nano-Carbon Composite Materials Network”

Funding: COST Action, European Union-Horizon 2020 Programme
Partners: 31 participating countries, chaired by the Karlsruhe Institute of Technology. IMDEA Materials Institute is one of the representatives of Spain.
Duration: 2016-2020
Principal Investigator: Dr. J. P. Fernandez

MultiComp is a COST Action designed to bring together theorists, experimentalists and industrialists in the field of nano-carbon materials technology. Although carbon nanotubes, graphene and few-layer graphene have been used to improve the properties of composite materials, two main problems remain to be solved before these composite materials can realize their full potential: (1) adequate dispersion of the nano-carbon reinforcement material, and (2) strong enough interfacial bonding between the nano-carbon reinforcement elements and the composite matrix. In addition to making modified Multi Walled Carbon Nanotubes (MWNTs) such as branched-MWNTs, the
Action will explore other possibilities of strengthening composites by integrating few-layer graphene; theoretical modelling of these nano-carbons and composites; development of new composite materials with electronic and multi-functional properties. This Action will provide an ideal platform, especially via short-term scientific exchanges, for permanent established researchers, post-doctoral workers and early-career investigators to enhance their research-related skills as well as their innovation and enterprise skills in this international network involving both academic and business enterprises.

**LIGHTIMP**

"X-ray computed tomography assessment of CNT-based CFRP damaged by impact lightning"

**Funding:** Tortech Nano Fibres  
**Duration:** 2016  
**Principal Researchers:** Dr. F. Sket

The main goal of LIGHTIMP is to analyse, by means of X-ray computed tomography (XCT), the damage generated by lightning impact on carbon fibre reinforced polymers (CFRP) laminates. The laminates’ surfaces will be protected by different amounts of high performance carbon nanotubes (CNT) veils and the typical copper mesh. The CFRP laminates will be first subjected to lab controlled lightning impact and the impacted laminates inspected by XCT. This non-destructive three-dimensional technique allowed observing and quantifying the damage generated at the surface and in the interior of the laminates and quantitatively compare the damage generated in the different laminate configurations.
**HIGHRATE**
“Mechanical behaviour of advanced high strength steels at high strain rates”

Funding: China Scholarship Council  
Duration: 2016-2020  
Principal Researchers: Dr. I. Sabirov

This main objective of this project is to study high strain rate mechanical behaviour of novel Advanced High Strength Steels (AHSS). The results of these investigations will greatly contribute to understanding of mechanical behaviour of the AHSS and help to reduce the dimensions of the AHSS components used in the automotive industry, and subsequently to reduce the weight of the cars while maintaining or improving their safety.

**CRASHING II**
“Front fuselage crashworthiness modelling”

Funding: Airbus Defense & Space  
Duration: 2016-2017  
Principal Researchers: Dr. C. S. Lopes

The CRASHING II project is the follow up of the Clean-sky CRASHING project and is focused on the modelling and simulation of the crashworthiness of an aircraft front fuselage using numerical composite material models developed in the initial project. The cabin model will be simulated in different crashing scenarios to evaluate its safety performance and provide design guidelines for future configurations.
NABISCO
“Integration of carbon nanotubes fibres in structural composites”

Funding: China Scholarship Council
Duration: 2016-2020
Principal Researchers: Dr. J. J. Vilatela

The main goal of NABISCO project is the development of strategies to integrate macroscopic fibres and films of CNTs into structural laminate composites. The aim is to improve the mechanical properties of traditional fibre-reinforced polymer composites, while providing them with new functions derived from the unique yarn-like structure of CNT fibres and the low dimensionality of their constituents.
Other ongoing research projects in 2016 at IMDEA Materials Institute were:

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

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

**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 Centre for Numerical Methods in Engineering (CIMNE), Project Coordinator) and IMDEA Materials Institute  
**Duration:** 2015-2017  
**Principal Investigator:** Dr. D. Y. Wang

**FUTUREALVE** “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

**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
MICROFRAC “Visualization and modelling of fracture at the microscale”

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

ADVANSEAT “Modular concept for 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

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

HIPREP “High Performance Reinforced Fire-retardant Polymers”

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

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
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. M. T. Pérez-Prado

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

CRIRCEM “Development of innovative materials for the cutting tool industry”

Funding: China Scholarship Council
Duration: 2015-2019
Principal Researchers: Dr. A. García-Junceda

CRISTAL “Corrosion resistant Zn-Al hypoeutectic alloys”

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

EXTRECP “Crystal Plasticity modelling under extreme conditions”

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

CRASHING “Characterisation 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: 2013-2016
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. F. Sket and Dr. C. González

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

Funding: Industria de Turbo Propulsores S.A. (ITP)
Duration: 2014-2017
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: 2014-2017
Principal Investigator: Dr. C. S. Lopes
EPISIM “Simulation of epitaxial growth”

Area: Asia / Pacific
Duration: 2014-2016
Principal Investigator: Dr. J. P. Balbuena

ONLINE-RTM “Online NDT RTM inspection in composites”

Funding: Centre for Industrial Technological Development (ESTEVEA CIEN programme), Spanish Ministry of Economy and Competitiveness and Airbus Operations S.L.
Duration: 2014-2016
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: 2014-2018
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: 2014-2018
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. M. Monclús

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

MICROMECH “Microstructure based material mechanical models for superalloys”

Funding: Clean Sky Joint Undertaking, EU Seventh Framework Programme for Research (FP7)  
Partners: IMDEA Materials Institute  
Duration: 2013-2016  
Principal Researcher: Dr. J. Segurado

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. A. Sarikov
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 Projektmangement (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 fibre-reinforced polymers”

Funding: Marie Curie Action- CIG, European Union-7th Framework Programme
Duration: 2013-2017
Principal Investigator: Dr. R. Guzmán de Villoria
ECOPVC “Eco-friendly fire retardant PVC nanocomposites”

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

HOTNOMECHE “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: 2012-2016
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
SIMET “Numerical simulation for metallic fragments impact on composite solutions”

Funding: AIRBUS OPERATIONS S.L. (Spain)
Duration: 2015-2016
Principal Investigators: Dr. C. González

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

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

Funding: Transport, European Union-7th Framework Programme
Partners: Consortium of 57 European partners from 18 countries coordinated by AIRBUS OPERATIONS GmbH
Duration: 2008-2016
Principal Investigator: Prof. J. LLorca
6.1. Publications [87]
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dissemination of results
6.1. Publications


91. X. Zhao, S. de Juan, F. Reyes-Guerrero, Z. Li, J. LLorca, D. Wang. Effect of N,N’-diallylphenylphosphoricdiamide on ease of ignition, thermal decomposition behavior and mechanical


6.2. Book Chapters


6.3. International Conferences

6.3.1. Invited and Plenary talks


20. “Multiscale computational mechanics of structural materials: composites & metals”, J. LLorca, Biomedical Engineering and Regenerative Medicine Summer School, National University of Ireland, Galway, Ireland, August 2016.


6.3.2. Regular contributions


22. “Design and characterisation of novel duplex stainless steels processed by field-assisted hot pressing”, A. García-Junceda, M. Rincón, J. M.


Conference (EMMC 2015), Brussels, Belgium, September 2016.


41. “CNT fiber-based multifunctional composites: the understanding the effect of the polymer infiltration on its mechanical and electrical properties”, B. Mas, A. Monreal-Bernal, J. J. Vilatela, ICNN4 - 4th International Conference on Nanomechanics and Nanocomposites, Vicenza, Italy, September 2016.


45. “Room temperature ferromagnetism in non-magnetic pure metals induced by severe plastic deformation”, C. M. Cepeda-Jiménez, A. Hernando, M. T. Pérez-Prado, 2016 EMI International Conference, Metz, France, October 2016.


6.3.3. Membership in Organising Committees


4. 17th European Conference on Composite Materials. C. S. Lopes and C. González. (Co-Organizers of the sessions on Novel composite microstructures: design and/or prototyping, on Dynamic Loading – Impact, Crash, Blast and on Ground-Based Transportation). Munich, Germany, June 2016.


6.4. Hosting and organisation of international Conferences and Workshops

One international conference and two international workshops were organised by IMDEA Materials Institute in 2016. Those events were held at the institute, taking advantage of the facilities available in our building.

One of the conferences was an initiative of a group of friends and colleagues to honor Prof. Subra Suresh on occasion of his sixtieth birthday. Over 150 representatives of global research, gathered around Professor Subra Suresh, President of Carnegie Mellon University, to discuss about interdisciplinary of research in Materials, Mechanics, Engineering and Medicine.

1. **7th International Conference on Composites Testing and Model Identification**, C. Gonzalez and C. S. Lopes (Chairmen), April 2015

2. “**Testing and Characterisation of Composite Materials**” - Seminar and Demonstration INSTRON ELECTROPULS, June 2016

3. “**Research, Innovation and Leadership at the Crossroads of Science, Engineering and Medicine**” honoring Prof. Subra Suresh on his sixieth birthday, Javier LLorca, Ming Dao, Lei Lu and Upadrasta Ramamurty (Chairs), June 2016

*Figure 5. Form left to right, Prof. Lei Lu, Prof. Ming Dao, Prof. Upadrasta Ramamurty, Prof. Subra Suresh, Prof. Javier Llorca and Prof. Jimmy Hsia during the Conference to honor Prof. Subra Suresh on his sixieth birthday at IMDEA Materials Institute.*
6.5. Invited Seminars and Lectures


2. “Multiscale Virtual Analysis of Composites: from microscale to non-conventional structural designs”, C. S. Lopes, NASA Langley Research Centre (LaRC), Langley, USA, February 2016.

3. “Multiscale Virtual Analysis of Composites: from microscale to non-conventional structural designs”, C. S. Lopes, University of South Carolina, Columbia, USA, February 2016.


6. “Multiscale modelling of structural materials: roadmaps for virtual testing of composites & metallic alloys”, J. LLorca, State Key Laboratory of High Performance Complex Manufacturing, College of Mechanical and Electrical Engineering, Central South University, Changsa, China, May 2016.


8. “A multiscale modelling strategy for virtual design of composites metallic materials: application to Ni-based superalloys”, J. LLorca, School of Materials Science, Northwestern Polytechnical University, Xi’an, China, May 2016.

9. “High temperature mechanical performance of metallic and metal-ceramic nanoscale multilayers”, J. LLorca, State Key Laboratory for the Mechanical Behavior of Materials, Xi’an Jiaotong University, Xi’an, China, May 2016.


15. “New approaches to impart flame retardancy to polymers”, D. Y. Wang, Xi’an Jiaotong University, Xi’an, China, July 2016.


19. “Some ideas on fire retardancy of polymeric materials”, D. Y. Wang, Zhejiang University, Hangzhou, China, October 2016.


22. “Using nanoindentation to assess slip and twinning activity in Mg between RT and 300 ºC”, J. M. Molina-Aldareguia, Northwestern Polytechnic University, Xi’an, China, November 2016.

23. “Micro and Nanomechanical testing oriented to fast material design”, J. M. Molina-Aldareguia, Central South University, Changsa, China, November 2016.


6.6. Seminars

1. “Nanoscale engineering and electrochemical approaches to next-generation energy storage”, Dr. Vinodkumar Etacheri (from Purdue University). January 2016.


17. “High strength Copper-Niobium nanomaterials”, Dr. Sezer Özer in (from University of Illinois at Urbana-Champaign). May 2016.


19. “Molecular engineering of materials for high performance and stable perovskite solar cells”,
Prof. Shahzada Ahmad (from Abengoa Research). May 2016.


24. “Bulk nanostructured materials processed by severe plastic deformation. From fundamentals towards applications”, Dr. Alexander Zhilyaev (from Institute for Metals Superplasticity Problems of Russian Academy of Science). July 2016.


27. “Gradient Effects in fracture and damage”, Dr. Emilio Martínez Pañeda (from Technical University of Denmark). October 2016.


6.7. Fellowships

1. AMAROUT EUROPE Programmes (I and II), Marie Curie Action (PEOPLE-COFUND), European Union, 7th Framework Programme
   - Call 2016: Dr. S. Daziri, Dr. S. Haouala, Dr. X. Wen
   - Call 2015: Dr. M. Haranczyk, Dr. A. Moitra
   - Call 2014: Dr. V. Babu

2. Ramon y Cajal Programme, Spanish Ministry of Economy and Competitiveness
   - Call 2014: Dr. J. J. Vilatela
   - Call 2013: Dr. C. S. Lopes, Dr. M. Haranczyk
   - Call 2012: Dr. D. Y. Wang
   - Call 2011: Dr. I. Sabirov

3. Postdoctoral Fellowship Programmes, Spanish Ministry of Economy and Competitiveness
   - Call 2015: Dr. V. Etacheri, Dr. A. Baluch
   - Call 2013: Dr. F. Sket

4. China Scholarship Council
   - Call 2016: C. Fu, Y. Ou, X. Peikang, J. Zhang
   - Call 2015: J. Li, N. Li, X. Deng, L. Zhang, J. Wang
   - Call 2014: C. Wang
   - Call 2013: Y. Pang, Y. Lingwei
   - Call 2012: Y. Chen, X. Zhao

5. Training University Lecturers (FPU) Programme, Spanish Ministry of Education, Culture and Sport
   - Call 2015: B. Belión
   - Call 2014: L. C. Herrera

6. Predoctoral Fellowships Programmes, Spanish Ministry of Economy and Competitiveness
   - Call 2013: A. Palomares

7. Youth Employment Programme, Spanish Ministry of Economy andCompetitiveness
   - Call 2014: C. Andradas, J. Castro, M. Cejuela, H. Mora

8. Youth Employment Programme, Madrid Regional Government
   - Call 2016: A. Doñoro, A. Larrañaga, J. de la Vega, A. Martín
   - Call 2015: F. Fernández, N. Pérez

9. Youth Employment Programme – predoctoral researchers, Madrid Regional Government
   - Call 2016: S. Lucarini, C. Gutierrez
6.8. Awards

1. Fellow of the Royal Society of Chemistry
   - Dr. D. Y. Wang

2. Elected, Board of Directors of the Society of Engineering Science
   - Prof. J. Llorca

3. 2016 Thesis talk award, University Carlos III of Madrid
   - Marcos Jiménez

4. 2016 young investigator award, European Society of Composite Materials
   - Dr. J. J. Vilatela

5. Fellow of the Leibniz Institute of Polymer Research Dresden
   - Dr. D. Y. Wang

6.9. Institutional Activities

- Member of the European Materials Modelling Council (EMMC).
- Member of the European Energy Research Alliance (EERA AISBL).
- Member of the Executive Committee of the Spanish Association for Numerical Methods in Engineering (SEMNI).
- Council member of the International Association for Computational Mechanics (IACM).
- 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).
- Local Contact Point of the EURAXESS pan-European initiative.
- Technical Secretariat of the Spanish Technological Platform of Advanced Materials and Nanomaterials (MATERPLAT).
- Member of the Board of Directors of the Spanish Association of Composite Materials (AEMAC).
- Member of the Spanish Aerospace Platform.
- Member of the Spanish Technological Platform for Advanced Manufacturing.
- 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).
6.10. Outreach


- Training on Materials for aerospace applications. Board of European Students of Technology (BEST).

- Collaboration with Formula Student UC3M team.

- Participation in the “XV Semana de la Ciencia”, promoted by Fundación Madri+d.

- Participation in the “European Researchers’ night Madrid 2016”, promoted by Fundación Madri+d.

- Organisation of primary and secondary school visits to IMDEA Materials Institute.

6.11. Theses

6.11.1. PhD Theses

“Dual scale flow during vacuum infusion of composites: experiments and modelling”
Student: Joaquim Vila
Technical University of Madrid
Advisor: Dr. C. González and Prof. J. LLorca
Date of defense: February 2016

“Atomistic modeling of Ge damage accumulation, amorphization and solid phase epitaxial regrowth”
Student: José Luis Gómez
Technical University of Madrid
Advisor: Dr. I. Martín-Bragado and Dr. J. Segurado
Date of defense: January 2016

“Multiscale analysis of the mechanical behaviour of needle-punched nonwoven fabrics”
Student: Francisca Martínez
Technical University of Madrid
Advisor: Prof. J. LLorca and Dr. C. González
Date of defense: February 2016

“Multifunctional layered double hydroxide (LDH) based epoxy nanocomposites”
Student: Ehsan Naderi Kalali
Carlos III University
Advisor: Dr. D. Y. Wang
Date of defense: January 2016

“Coupled nonlinear Ginzburg-Landau and mechanics model for martensitic transformations in polycrystals”
Student: Guanglong Xu
Technical University of Madrid
Advisor: Dr. Y. Cui and Prof. J. LLorca
Date of defense: February 2016

“Assessment of the eutectic trough and properties of a multiphase alloy in the NiAl-Cr-W system”
Student: Arcadio Varona
Carlos III University
Advisor: Dr. S. Milenkovic
Date of defense: September 2016
6.11.2. Master/Bachelor Theses

“Comportamiento mecánico de una aleación Al-Mg-Si de grano ultrafino”
Student: Edurne Gomez
Technical University of Madrid
Advisor: Dr. I. Sabirov
Date of defense: July 2016

“Effect of grain refinement on mechanical behavior and biaxial stretching formability of Al 5083 alloy”
Student: Miguel Angel Valdes
Technical University of Madrid
Advisor: Dr. I. Sabirov
Date of defense: July 2016

“Preparación de redes poliméricas inteligentes”
Student: Luis Mario Martín
Carlos III University
Advisor: Dr. J. P. Fernández
Date of defense: October 2016

“Diseño y caracterización de aceros inoxidables dúplex consolidados mediante la técnica de compactación en caliente asistida por campo eléctrico”
Student: Víctor Gómez
Rey Juan Carlos University
Advisor: Dr. A. García-Junceda
Date of defense: July 2016

“Estimación del efecto de las tierras raras en el comportamiento del magnesio mediante ensayos de indentación y modelos de plasticidad cristalina”
Student: Javier Sánchez
Technical University of Madrid
Advisor: Dr. J. Segurado
Date of defense: June 2016

“Composite sensors based on CNT fibres”
Student: Sergio Frutos
Technical University of Madrid
Advisor: Dr. J. J. Vilatela
Date of defense: August 2016

“High performance flame retardant polymer foams as new thermal insulators”
Student: Jose Manuel Rodriguez
Carlos III University
Advisor: Dr. D. Y. Wang
Date of defense: July 2016

“Preparation and properties of high performance halogen free flame retardant thermoplastics”
Student: Javier Rosas
Carlos III University
Advisor: Dr. D. Y. Wang
Date of defense: July 2016
6.12. Internships / Visiting students

“Developing nanostructured TiO2 electrodes for Li-ON batteries”
Student: Leyre Maroto
Advisor: Dr. V. Etachery
Visiting student from: Rey Juan Carlos University
Period: August 2016-November 2016

“In-plane characterization and fracture toughness of tri-axially braided composite materials”
Student: Jeroen Knippenberg
Advisor: Dr. C. González, Dr. C. S. Lopes and A. García
Visiting student from: Eindhoven University of Technology
Period: February 2016-June 2016

“Conductividad eléctrica a través del espesor en láminas delgadas de fibra de carbono con adición de nanotubos de carbono”
Student: Héctor Bautista
Advisor: Dr. C. González and M. Herráez
Visiting student from: Technical University of Madrid
Period: February 2016-July 2016

“Preparación de laminados híbridos mediante el esparcimiento de mechas. Fabricación de paneles”
Student: Jonnathan Santos
Advisor: Dr. C. S. Lopes, Dr. C. González and M. Herráez
Visiting student from: University of Girona
Period: July 2016

“Tomography of single ply tri-axially braided composite panels to obtain the mesh of the unit cell”
Student: Bas Van Den Beucken
Advisor: Dr. C. S. Lopes, Dr. C. González and A. García
Visiting student from: University of Technology Eindhoven
Period: August 2016-December 2016

“Micromechanical testing of interfaces of a new composite material for high temperature applications. Nanoindentation test for measuring the strength of interfaces of composite material at RT and different aging conditions”
Student: Xiaochen Li
Advisor: Dr. C. S. Lopes and Dr. C. González
Visiting student from: University of Southern California
Period: September 2016-December 2016

“Nano-architecture and materials design”
Student: Rubén Lebron
Advisor: Dr. R. Guzmán de Villoria
Visiting student from: Carlos III University
Period: February 2016-April 2016

“Nano-architecture and materials design”
Student: Mario Jañez
Advisor: Dr. R. Guzmán de Villoria
Visiting student from: Rey Juan Carlos University
Period: April 2016-June 2016

“Nano-architecture and materials design”
Student: Daniel Berlanga
Advisor: Dr. R. Guzmán de Villoria
Visiting student from: Technical University of Madrid
Period: June 2016-August 2016

“Data-driven discovery of advanced materials. Towards the design of organic molecular-cages-based materials”
Student: Raúl Pérez
Advisor: Dr. M. Haranczyk
Visiting student from: University of Granada
Period: June 2016-September 2016

“Characterization of micropillar behaviour during fracture”
Student: Valerio Carollo
Advisor: Dr. J. Molina
Visiting student from: IMT School for Advanced Studies Lucca
Period: February 2016-August 2016
“Life improvement of TiAl blades for new generation of aeroengines”
Student: Cristina Gutierrez
Advisor: Dr. J. Molina
Visiting student from: University of Oviedo
Period: July 2016-September 2016

“Study of deformation mechanism of Mn11 Magnesium alloy by slip trace analysis”
Student: Cristina Prado
Advisor: Dr. M. T. Perez-Prado
Visiting student from: University of Varsovia
Period: June 2016-September 2016

“Numerical methods for the simulation of explicit contact: application to ice impact”
Student: Ignacio López
Advisor: Prof. I. Romero
Visiting student from: Technical University of Madrid
Period: June 2016-August 2016

“Conformabilidad de aceros avanzados de alta resistencia (AHSS) obtenidos vía Q&P”
Student: Alberto Cabo
Advisor: Dr. I. Sabirov
Visiting student from: Technical University of Madrid
Period: March 2016-June 2016

“Desarrollo de un modelo micromecánico para la simulación de mecanismos de fluencia en Inconel 718”
Student: Eva Mª Andrés
Advisor: Dr. J. Segurado
Visiting student from: Technical University of Madrid
Period: April 2016-July 2016

“Visualization of fracture at the microscale”
Student: Sandra Colomina
Advisor: Dr. A. Weck
Visiting student from: Technical University of Madrid
Period: June 2016-July 2016

“Fabricación de materiales compuestos y caracterización no destructiva por ultrasonidos y tomografía de rayos X”
Student: Javier Bedmar
Advisor: Dr. F. Sket
Visiting student from: Rey Juan Carlos University
Period: June 2016-August 2016

“Characterization of a piezoresistive carbon nanotube fiber based sensor for structural health monitoring”
Student: Sergio Frutos
Advisor: Dr. J. J. Vilatela
Visiting student from: Technical University of Madrid
Period: July 2016- August 2016
“Micromechanics of CNT fibres”
Student: Hugo Solera
Advisor: Dr. J. J. Vilatela
Visiting student from: Universidad Iberoamericana
Period: May 2016-August 2016

“Fabrication of flexible energy storage devices based on nanostructured carbon electrodes”
Student: Silvia Caminero
Advisor: Dr. J. J. Vilatela, Dr. E. Vinod and Dr. V. Etacheri
Visiting student from: Autonomous University of Madrid
Period: June 2016-September 2016

“Effect of phosphorus-containing flame retardant on RTM6/Carbon fiber composite: thermal stability, flammability and mechanical properties”
Student: Juan Picón
Advisor: Dr. D. Y. Wang
Visiting student from: Technical University of Madrid
Period: January 2016-March 2016

“From functional chemicals to high performance fire safety polymer-based composites”
Student: Alejandro Jimenez
Advisor: Dr. D. Y. Wang
Visiting student from: Rey Juan Carlos University
Period: January 2016-June 2016

“Novel Synthesis of hierarchical porous double-shelled hollow hybrid nanomaterials to reinforce multiple properties of flexible polyvinyl chloride film”
Student: Chengcheng Huang
Advisor: Dr. D. Y. Wang
Visiting student from: Technical University of Madrid
Period: January 2016-June 2016

“Polymer nanocomposites”
Student: Leijin Liu
Advisor: Dr. D. Y. Wang
Visiting student from: Technical University of Madrid
Period: February 2016-June 2016

“Synthesis and polymer processing”
Student: Xueyuan Gao
Advisor: Dr. D. Y. Wang
Visiting student from: Technical University of Madrid
Period: February 2016-July 2016

“Preparation of PU foam”
Student: Asunción Molina
Advisor: Dr. D. Y. Wang
Visiting student from: Complutense University of Madrid
Period: June 2016-August 2016
“Functional LDH and its application in polymers”
Student: Sara Montero
Advisor: Dr. D. Y. Wang
Visiting student from: Carlos III University
Period: June 2016-August 2016

“Investigation of fire safety behaviors of chemical materials”
Student: Daniel Fernández
Advisor: Dr. D. Y. Wang
Visiting student from: Rey Juan Carlos University
Period: June 2016-August 2016

“Fire testing of polymers, preparation of polymer nano-composites and polymer blending”
Student: Marina García Carrión
Advisor: Dr. D. Y. Wang
Visiting student from: Complutense University of Madrid
Period: July 2016-September 2016

“Fiber reinforced PLA and its fire retardancy”
Student: Adriana Pérez
Advisor: Dr. D. Y. Wang
Visiting student from: Autonomous University of Madrid
Period: September 2016-October 2016

“Fire retardancy of P-containing based polymers”
Student: Ceren Suer
Advisor: Dr. D. Y. Wang and N. Pérez
Visiting student from: Yildiz Technical University
Period: November 2016

“Microstructural and in situ mechanical characterization of γ-TiAl alloy”
Student: Raúl García
Advisor: A. Palomares and Dr. E. Ruiz Navas
Visiting student from: Carlos III University
Period: November 2015-September 2016

“Damage tolerance of dispersed plies laminates under low impact velocity: Simulation and validation of an optimisation method”
Student: Théophile Gaudin
Advisor: Dr. González and Dr. C. S. Lopes
Visiting student from: École Polytechnique fédérale de Lausanne
Date: September 2015-April 2016

“Novel duplex stainless steels processed by a powder metallurgy route involving field-assisted sintering technique”
Student: Coral Henar Díaz
Advisor: Dr. A. García-Junceda
Visiting student from: Carlos III University
Date: November 2015-October 2016
6.13. Courses

“Hierarchical Composites”
Master in Composite Materials, Technical University of Madrid and Airbus
Professor: Dr. J. J. Vilatela

“Non conventional Composites”
Master in Composite Materials, Technical University of Madrid and Airbus
Professors: Prof. J. L lorca, Dr. J. J. Vilatela, Dr. R. Guzmán de Villoria, Dr. I. Sabirov

“Metal-matrix Composites”
Master in Composite Materials, Technical University of Madrid and Airbus
Professor: Dr. I. Sabirov

“Simulation Techniques and Virtual Testing”
Master in Composite Materials, Technical University of Madrid and Airbus
Professors: Dr. C. González, Dr. J. Segurado, Dr. C. S. Lopes, Dr. D. Garijo, Dr. J. Múgica

“Simulation in Materials Science and Engineering”
Master in Materials Engineering, Technical University of Madrid
Professors: Prof. J. Llorca, Dr. C. S. Lopes, Dr. C. González, Dr. Y. Cui, Dr. M. Haranzcyk

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

“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, Dr. C. S. Lopes

“Advanced Strength of Materials”
Master of Industrial Engineering, Technical University of Madrid
Professor: Prof. I. Romero

“Mechanics of Composite Materials”
Master in Mechanics, Saint Petersburg State University
Professor: Dr. I. Sabirov

“Thermal and Thermomechanical Testing of Materials”
Master in Materials Science and Engineering, Carlos III University of Madrid
Professor: Dr. S. Milenkovic

“Nanomaterials”
Master in Materials Science, Carlos III University of Madrid
Professor: Dr. J. J. Vilatela

“Advanced Composite Materials”
Master in Materials Science, Carlos III University of Madrid
Professors: Dr. C. S. Lopes, Dr. J. M. Molina
7.1. Advanced materials for multifunctional applications [116]

7.2. Muesli: an open source library for the simulation of materials [120]

7.3. Design of metallic powders for additive manufacturing [122]
New challenges call for new materials and integration methods

Multifunctionality is a paradigm change in Materials Science and Engineering that aims at producing new materials and structures that can carry out multiple functions simultaneously. This quest is closely related to current technological trends, including the development of flexible optoelectronic devices, smart textiles, more efficient energy management and the electrification of transport. Electric vehicles, for example, require advanced energy storage solutions that are also safe, based on lightweight materials and compatible with mass-production methods. These challenges call for a new generation of advanced materials developed by multidisciplinary teams.

The 34 researchers in the Programme on Advanced Materials for Multifunctional Applications at IMDEA Materials Institute provide a wide expertise in design and synthesis of nanomaterials and their integration in devices and composites with combined fire-safety, high-performance mechanical properties and efficient energy management, amongst other properties.

Figure 1. Multifunctional requirements envisaged in the next generation of electrical vehicles
In the context of composite safety, the activities of the Programme include the development of eco-benign fire retardant materials and high performance environment-friendly polymers and composites using novel bio-based polymers and innovative synthetic chemistry and advanced processing methods. Our researchers have studied, for example, the synthesis, fire behaviour and mechanical properties of epoxies with halogen-free flame retardants [1].

Since mid-2016, researchers at IMDEA Materials Institute have also been active in the fabrication of new electrodes for ultrafast Li/Na ion storage based on new architectures combining advanced inorganic materials and porous nanocarbon scaffolds produced in-house (Figure 3 a-b), and using chemical methods to tailor interfaces for efficient charge storage and reduced fire hazard. There is rapid progress in the assembly and evaluation of batteries (Figure 3c) under operational conditions.

Nanocarbons are ideal elements in electrodes used for charge storage or charge transfer. Assembled as macroscopic fibres of long aligned CNTs, these materials combine very high electrical conductivity, chemical resistance and a large porosity to host other phases. Furthermore, their yarn-like network structure implies that they can simultaneously play the role of current collector and reinforcement in a composite. Work in the Programme aims at using CNT fibres in various structural energy managing composites. With reversible Li-ion intercalation (Figure 3d) capacity similar to commercial graphite anodes and toughness superior to that of Kevlar, the starting point for this work is encouraging [2].
Figure 3. TEM images of (a) CNT and (b) TiO₂ nanosheet-CNT hybrid electrodes (c) photograph and (c) electrochemical performance of Li-ion battery containing CNT electrode.

Figure 4. Multifunctional electrodes based on high performance carbon nanotubes fibres.
The growing list of required functions in applied materials and the ever-increasing library of molecular or nano building blocks point to the use of computational and data-driven materials discovery as another key element in the development of multifunctional materials. The research group at IMDEA Materials Institute dedicated to this topic develops strategies to enable in silico identification of the best molecules or materials for a given application at minimal computational costs. Their tools provide a) structure prediction and material database enumeration, b) high throughput structure characterization and property prediction and c) accelerated structure searchers using advanced algorithms.

In the context of advanced porous materials, for example, these techniques have been used to discover high performing material for noble gas separations [3] while entirely new approaches are being developed to enable computer-aided design of tunable molecular materials.

References


Muesli: an open source library for the simulation of materials

Computational solid, fluid, and structural mechanics pivots on simulation codes that approximate the solution of (initial) boundary value problems whose equations are too complex to be solved analytically. These equations include balance laws, sometimes constraints and, invariably, material models. The latter consists of software implementations of the constitutive relations that describe the behaviour of materials under all possible loading paths.

Despite their presence in all simulation codes for mechanics, material models are currently not shared, and this slows down the progress of research. Each company and research institution involved in this area of research is thus forced to develop its own set of software routines for standard materials, debug, verify and test them, before they are linked to its own large scale code.

In addition, new computational material models presented in scientific publications are invariably limited to the use of the developers. This hinders its adoption by the international scientific community which should go again through the costly and repetitive process of implementing, debugging, verifying, and testing to use these models.

As yet another research centre that routinely goes through the aforementioned software development cycle, IMDEA Materials institute, and more precisely its Computational Solid Mechanics group, has analysed this problem and proposed a solution. MUESLI, a Material UnivErsal Library, is an open source collection of material models at the continuum level launched in May 2016 and available in our web (http://materials.imdea.org/research/simulation-tools/muesli/). MUESLI encompasses continuum models for solid, fluid, and thermal mechanics in a C++, object oriented library designed for easy extension and flexible link with existing simulation codes. This library can be employed by research centres to explore new material models and by companies to implement their own specific material products.

MUESLI already includes the most commonly used continuum material models for solid, fluid, and thermal analyses. In particular, it has versions for small strain elastic, viscoelastic, elastoplastic, and viscoplastic materials, large strain hyperelastic and elastoplastic materials, Newtonian fluids, small strain strongly coupled materials, and Fourier type thermal conductors. Adding new material models is relatively simple because, in contrast with other implementations based on Fortran 77 or C, MUESLI makes use of high level
abstractions afforded by C++. As a result, the implementations in MUESLI resemble the symbolic expressions used in the mathematical description of the models implemented.

The material models implemented in MUESLI can be used in any simulation code, simply by developing a short interface. By doing so, and with a minimal amount of work, researchers can tap onto the large, and growing, database of material models implemented in the library. MUESLI can also be linked to commercial simulation codes and an interface is already available for Abaqus and LS-DYNA. Thus, the same material models can be employed in different research and commercial simulation programs, speeding up development time and technology transfer to companies.

MUESLI has some very useful features from the point of view of software design. In addition to a well-defined structure based on object oriented classes, and high-level syntax, the code includes several tools for self-testing. Thus, all material models in the library are verified for self consistency, and potential bugs can be easily found in complex implementations.

MUESLI has been created at the institute with the goal that researchers and companies which develop and use material models can share them. The library is distributed under a GPL 3.0 open source license, and includes documentation for the implemented models. True to its open source philosophy, the MUESLI project accepts external contributions, aiming to become a standard and useful tool for the material simulation community.

References

Design of metallic powders for additive manufacturing

Additive manufacturing (AM), often termed 3D printing of metals, is emerging as a new paradigm in the fabrication of metallic parts. Although still only a few parts made with this technology are being commercialized, it is envisioned that AM will impact significantly the fabrication of metallic components, allowing for more freedom in design, weight savings, waste reduction and added multifunctionalities. Applications where AM could replace existing manufacturing methods include, for example, metallic implants, which could be customized for each individual patient. Vast efforts are being made worldwide to explore further applications of this technology in all industrial sectors.

The Physical Metallurgy group at IMDEA Materials Institute has launched a new research line on the development of new feedstock for AM. In particular, a gas atomization process is currently being optimized to produce powders of pure metals and alloys with the right composition, morphology and size distribution that could then constitute the raw material for selected laser melting (SLM), electron beam melting (EBM) or laser metal deposition (LMD). Processing is carried out using a horizontal gas atomizer (Fig. 1), where bulk material is melted using an arc melting furnace and then atomized using a jet and cone nozzle type. Process optimization includes tailoring the melt temperature, melt flow, gas pressure and vacuum levels for each metal powder.

Figure 1. Gas atomizer unit available at IMDEA Materials.
The powders thus fabricated are characterized using a combination of techniques such as electron microscopy (Fig. 2), X-ray diffraction and various rheology methods. The main aim is to obtain particles with spherical morphology and with sizes smaller than about 100 microns, that are endowed with good flowability and packing density (Fig. 3). The ultimate goal of this research is to develop new alloy compositions that are specifically targeted for additive manufacturing applications and which can, ideally, exhibit unique properties beyond reach in conventionally fabricated metals.

The Physical Metallurgy group is currently partnering other international institutions in several EU-funded consortia aimed at optimizing additive manufacturing processes for the aerospace and biomedical sectors. In particular, funding has been obtained in the frame of the CleanSky2 and M-era.Net calls to fabricate, respectively, Al alloys and ultrafine Fe and Ti based eutectics in powder form for AM. The CleanSky2 consortium (Alforama) is led by Lortek (Spain) and integrated also by a group of KU Leuven (Belgium); the M-era.Net consortium (ELAM) is led by the DLR Institute for Materials Research (Germany) and other members including several companies (Access, Bosch-Mahle, P&G Manufacturing, all located in Germany) and research institutions such as Wigner RCP (Hungary) and the Fraunhofer Society (Germany).
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