imdea materials institute

excellence as our technological key

annual report 2017

www.materials.imdea.org
Ignacio Romero
Director, IMDEA Materials Institute
March 2018

annual report
2017
www.materials.imdea.org
This year marks the tenth anniversary of the IMDEA project, and our Institute in particular. Ten years during which, in our case, we evolved from a one-man project backed by Madrid’s regional government, to a research institution of 116 people, dedicated to the study of the broad field of Materials Science.

After this initial period, it seems a good moment to reflect upon whether we have fulfilled to the mission given to us by our Board of Trustees. First, as this report shows, our scientific contributions and impact have grown steadily. During this year, for example, we have produced over 100 JCR journal articles and the number of citations for work done at the Institute, during the same period, is now over 2000. Second, we remain committed to bringing the best researchers to our centre, irrespective of their origin. In 2017, two new researchers joined the Institute to open new lines: one in hybrid optoelectronic materials and devices, the second in modelling and simulation of materials processing. Third, we strive to transfer the accumulated experience to industry and nearby academic institutions. During this same period, we have started nine new projects with companies from all over the world, while we witness a progressive growth in international recognition.

At ten years of age, IMDEA Materials Institute is full of life. A first sign of this impulse is that Prof. Javier LLorca, the former director of the Institute, decided that the momentum of the centre was strong enough that, as any other reputed scientific institution, its head should change regularly so that it can benefit from different contributions. Let me, in this my first foreword, thank Prof. LLorca in the name of all members of IMDEA Materials Institute for his work and leadership during the past years.

A second sign of the current impulse in the Institute is the launch, during 2017, of three Strategic Initiatives (Strategic Emerging Technologies), proposed by interdisciplinary teams within the Institute, funded internally, and designed to shape our research in upcoming years. After much preparation, we agreed to push projects on additive manufacturing of metals, structural batteries, and smart manufacturing of composites. These projects have injected new activities into the three horizontal programmes of the Institute and have, immediately, received interested attention from our strategic industrial partners.

But these ten years are, hopefully, just the start of a long-term endeavour. Significant organisational and scientific challenges await, and it is our duty to anticipate them. We are committed to do our best, so that when the moment comes to celebrate the 20th anniversary we can conclude, as we do today, that the Institute has been able to grow and improve thanks to them.

words from the director...
about us

The IMDEA Materials Institute (Madrid Institute for Advanced Studies of Materials) is a non-profit research organisation promoted by the Regional Government of Madrid in 2007. The mission and vision of the Institute is based in three main pillars:

- **excellence** in materials science and engineering research
- **technology transfer** to industry to increase competitiveness and maintain technological leadership
- **attraction of talented** researchers from all over the world to Madrid to work in an international and interdisciplinary environment

The IMDEA Materials Institute has a **established international reputation in the areas of design, processing, characterisation, modelling and simulation of advanced materials** for applications in different industrial sectors with particular emphasis in transport and energy.

**Research Programmes: Fundamental and Applied**

- 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

**Societal Challenges**

- Automotive
- Aeronautics
- Defence & Security
- Energy

**Strategic Partners**

- ITP Aeronaútica
- Airbus
- Airbus Defence & Space
- Hidrolight
- Tolosa
The core strength of the Institute is its international research team, consisting of talented researchers from 16 different nationalities, which carries out new scientific discoveries in materials science, and foster the development of emerging technologies.

The facilities of IMDEA Materials Institute
The building and laboratories of IMDEA Materials Institute are located at the Scientific and Technological Park of the Technical University of Madrid in Tecnogetafe, Madrid.

- 2.640 m² of research labs
- 4 pilot plants
- Auditorium (200 people) and networking space for international Conferences and Workshops

State-of-the-art laboratories to manufacture, characterise and simulate advanced materials and nanomaterials, including their integration in lab scale prototypes and devices.

- 116 researchers
- 16 nationalities
- 50% PhDs
- 40% foreign researchers
- 16 research groups
CHAIRMAN OF THE FOUNDATION
Prof. Juan Manuel Rojo
Emeritus Professor
Complutense University of Madrid, Spain

VICE-CHAIRMAN
OF THE FOUNDATION
Excmo. Sr. D. Rafael van Grieken Salvador
Regional Minister of Education, Youth and Sports
Madrid Regional Government

PERMANENT TRUSTEES (REGIONAL
GOVERNMENT)
Excmo. Sr. D. Rafael van Grieken Salvador
Regional Minister of Education, Youth and Sports
Madrid Regional Government
Ilmo. Sr. D. Alejandro Arranz Calvo
General Director for Research and Innovation
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 (Madrild)

UNIVERSITIES AND PUBLIC
RESEARCH INSTITUTIONS
Prof. Antonio Hernando
Professor
Complutense University of Madrid, Spain
Prof. Paloma Adeva
Research Professor
Coordinator of the Materials Science and
Technology Area (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

SECRETARY
Mr. Alejandro Blázquez

VICE-CHAIRMAN
OF THE FOUNDATION
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
Emeritus 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

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

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

SECRETARY
Mr. Alejandro Blázquez

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

Prof. Trevor William Clyne
Professor
Cambridge University, UK

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. Judith L MacManus-Briscoll
Professor
University of Karslhuhe, Germany

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

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

Prof. Pedro Muñoz-Esquer
Independent consultant

Prof. Michael Ortiz
Professor
Polytechnic University of Catalonia, Spain

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

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

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

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

Prof. Mauricio Terrones
Professor
The Pennsylvania State University, USA
Talent attraction has been the key to the Institute’s success.

Open and transparent selection along with regular evaluation of principal investigators performed by an independent Scientific Council.

IMDEA Materials has created a multidisciplinary and international working environment to attract and maintain talented researchers from all over the world.

Career development at IMDEA Materials is acknowledged by the EU’s HR excellence in research seal.

Technology and knowledge transfer to society through talent transfer

24 defended PhD theses since 2007
64 ongoing PhD theses
The scientific excellence of the Institute is accredited by the evolution of the number of publications (JCR) and citations over the last ten years.

2017

- **29** keynote/invited talks
- **101** JCR papers
- **40** invited seminars
- **5** patents applied
- **1937** number of citations

![Graph showing the evolution of papers and citations from 2007 to 2017](image-url)
The unique scientific expertise and infrastructure of IMDEA Materials Institute enables its research groups to collaborate with national and international industry for the benefit of the Madrid’s region and its development as technological hub in Europe.

Companies which had active collaboration with IMDEA Materials during 2017
Research activities are performed in the framework of R&D projects and fellowships, which are funded either by regional/national/international agencies or through direct contracts with companies.

**2017**

- **International projects**: 61%
- **National projects**: 11%
- **Regional projects**: 11%
- **Contracts with industry**: 17%

<table>
<thead>
<tr>
<th>Year</th>
<th>R&amp;D projects</th>
<th>ERC projects running</th>
<th>R&amp;D contracts with companies</th>
</tr>
</thead>
<tbody>
<tr>
<td>2017</td>
<td>44</td>
<td>2</td>
<td>17</td>
</tr>
</tbody>
</table>
10 years of success

2007
- Launch of IMDEA Materials Institute

2008
- First European Project. MAAXIMUS

2009
- Temporary facilities at the Technical University of Madrid

2010
- Final site inauguration

2012
- First industrial R&D contracts

Temporary facilities at the Technical University of Madrid

The beginning of the final site construction
10 years' success indicators

- Over 600 JCR papers and 6,641 citations
- Participation in 41 EU projects
- Coordination of 11 EU projects
- Over 26 M€ funding attracted
- 116 researchers of 16 nationalities
- Over 60 R&D contracts with companies
- 24 defended PhD theses and 64 ongoing
Advanced Materials for Multifunctional Applications

- Synthesis and integration of nanomaterials and polymer-based multifunctional nanocomposites
- New materials and strategies for electrochemical energy storage and conversion
- Hybrid optoelectronic materials and sustainable lighting devices
- Computational and data-driven materials discovery

The Next Generation of Composite Materials

- Processing of high performance composites and nanocomposites. Recycling structural composites
- New frontiers of structural performance (impact, high temperature, mechanical...)
- Virtual testing and virtual processing of structural composites. Sensing and Industry 4.0
- Multifunctional capabilities (fire resistance, electrical, thermal, sensing, energy management, health monitoring...)

research 2017
Novel Alloy Design, Processing and Development

- Structural alloys: light alloys, high temperature alloys and high strength steels
- Characterisation of microstructure and mechanical behaviour
- Advanced Manufacturing: solidification and casting, physical simulation of metallurgical processes (rolling, forging, extrusion...)
- Additive manufacturing: powder design and fabrication, process optimisation
- Virtual processing and virtual testing of metallic alloys

Multiscale Characterisation of Materials and Processes

- 3D characterisation of materials (X-ray tomography and diffraction, SEM, TEM...)
- 4D characterisation: In-situ characterisation of deformation and processes across multiple length scales (750°C)

Integrated Computational Materials Engineering

- Virtual materials design, including virtual processing and virtual testing
- Materials modelling at different length and time scales
- Multiscale materials modelling
facilities

IMDEA Materials Institute has state-of-the-art laboratories to manufacture, characterise and simulate advanced materials and nanomaterials, including their integration in lab scale prototypes and devices.

Synthesis, processing and integration of materials

Metallic alloys
- Bulk processing techniques: casting by induction and arc melting, as well as a Gleeble physical simulator, furnished with fixtures suitable for rolling, extrusion, torsion, sintering, welding, and rapid solidification.
- Powders manufactured by gas atomisation and mechanical milling. Selective laser melting technology for additive manufacturing of metals (to be installed in 2018).

Polymer based composites and nanocomposites
- Liquid moulding processing: RTM resin transfer moulding, VI vacuum infusion, RFI resin film infusion and pultrusion.
- Prepreg lamination using vacuum bagging of autoclave and out-of-autoclave prepregs (OoA) or laminate hot-press moulding (<400°C).
- Semi-industrial equipment for compounding and injection moulding of thermoplastics.
- Integration of advanced nano-fillers.

Nanomaterials
- Synthesis and chemical modification of nanocarbons, inorganic materials, nanoporous semiconductors, thin films, zeolites and other nanomaterials.
- Evaporation equipment in controlled atmospheres, high-pressure reactors and in-house chemical vapour deposition systems.

Energy storage and conversion devices
- Synthesis and characterisation of nanostructured electrode materials for energy storage applications. Fabrication of composite electrodes and integrated in various types of rechargeable batteries (Li-ion, Li-S, Li-O₂, Na-ion, and hybrid batteries etc.).
- Fabrication and testing of nanocarbon-based electrodes and their integration with liquid and solid electrolytes to form large-scale (> 100 cm²) flexible supercapacitors.
- Integration of energy-storage functions in structural composites
- Fabrication (solvent-based deposition, physical vapour deposition, high temperature sintering ovens and hot plates) and characterization (solar simulators, incident photon-to-current conversion, electrochemical impedance spectroscopy and intensity-modulated photovoltage spectroscopy) of hybrid solar cells and thin-film organic solar cells.

Lighting devices
- Fabrication and characterisation of hybrid light-emitting diodes and thin-film lighting devices.
- Rack system consisting of 7 positions that are independently driven, while the luminance and chromaticity features are monitored over time via UV-VIS spectrophotometers coupled to integrated spheres.
- Station to measure spatial light distribution and temperature generation in a micrometre resolution over time.
- Rack system for measuring thin film lighting devices using different poling modes, while controlling luminance and chromaticity features over time using eye-corrected detectors
- Electrochemical impedance spectroscopy (EIS).
### Microstructural and chemical characterisation
- 3D microscopy at different length-scales, including X-ray tomography, 3D-SEM, 3D-EDS and 3D-EBSD in the FIB and 3D-TEM and 3D-EDS in the TEM.
- In-situ mechanical testing of mininaturised samples in the X-ray tomography system as well as in the SEM and TEM.
- In-situ processing studies in the X-ray tomography system, such as casting, infiltration and curing of polymer based materials.
- Raman spectrophotometer.

### Functional properties
- **Fire resistance**
  - Rapid laboratory scale tests for screening (micro-scale combustion calorimetry and oxygen index).
  - Dual cone calorimetry and UL94 Horizontal/Vertical Flame Chamber.

### Mechanical properties
- **Thermal**
  - DSC, TGA and Hot Disk Thermal Conductivity analyse. Thermal behaviour of mechanical properties, DMA and rheology. Horizontal and Vertical Flame Chamber.
  - Pushrod Dilatometer for the measurement of dimensional changes.

- **Electrochemical**
  - Electrochemical characterisation of energy storage devices (Li-ion, Li-S, Li-O2, Na-ion, and hybrid batteries). Simultaneous testing of 100 batteries can be performed using multichannel battery testers.

- **Simulation**
  - **Galvanostatic/potentiostatic cycling at various current densities.**
  - Single channel Zive SP1 electrochemical workstation is used for cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) study of batteries.

- **Photophysical**
  - UV-VIS absorption and emission spectrophotometers for solutions, thin films, and powders.
  - Integrating spheres to measure diffuse reflectance and photoluminescence quantum yields.
  - Electrochemical stations to perform static and time-resolved spectroelectrochemistry.
Advanced Materials for Multifunctional Applications

Goal and vision

The Programme on Advanced Materials for Multifunctional Applications at IMDEA Materials Institute combines expertise in design and synthesis of nano and molecular building blocks with 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.
High Performance Polymer Nanocomposites
Electrochemical Energy Storage, Nanomaterials
Multifunctional Nanocomposites
Hybrid Optoelectronic Materials and Devices
Computational and Data-Driven Materials Discovery
Main research lines

Synthesis and integration of nanomaterials (nanotubes, nanofibers and hybrids)
• 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.

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, nano coatings, etc.

Solar energy conversion schemes
• Advanced dye-sensitised solar cells: Pt-free counter-electrodes, new electrolytes, etc.
• Fabrication of flexible solar cells with non-conventional substrates.

Thin-film lighting technologies
• Development of perovskite-based lighting devices with a focus on new NPs and device architectures.
• Fabrication of efficient and stable white lighting devices based on new organic and organometallic emitters.
• Dual functional devices: Design of novel device architectures and components.

Bio-hybrid optoelectronics
• Design of elastomeric color down-converting materials based on fluorescent proteins.
• Fabrication and analysis of single-point lighting and display systems.
• Further development towards bio-diagnosis and bio-reactor applications.

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-O2.

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.
Projects in focus

**MOFMAP / Tailored metal-organic framework: from hybrid to multifunctional flame retardant polymer nanocomposites**

**Funding:** European Union, Horizon 2020 Programme (Grant Agreement 705365). Marie Skłodowska-Curie-IF

**Project period:** 2017 – 2019

**Principal Investigator:** Dr. Xiao-Lin Qi, Supervisor: Dr. De-Yi Wang

The main objective of this project is to develop a new generation of polymer-based multi-functional nanocomposites by combining functionalized Metal-Organic Frameworks (MOFs) and flame retardancy into polymeric matrices via an innovative approach. In this work, the intrinsic porosity of MOFs is employed to develop multifunctional polymer nanocomposites with enhanced performances for the first time. The Zn(II) or Cu(II) contained MOFs are chosen as the host framework, which are environmental friendly and the widely used unsaturated polyester is adopted as the polymer matrix. The new knowledge and new materials developed in this project have a great potential to be applied in developing a new generation of products in the fields of energy storage, construction, transportation, aerospace, etc.

**DFID / Dual-functional ionic-based devices: electroluminescence and photovoltaic responses in one**

**Funding:** Regional Government of Madrid, Talent attraction, modality 1 (Grant 016-T1/IND-1463)

**Project period:** 2017 – 2021

**Principal Investigator:** Dr. Rubén Costa

The R&D solid-state technologies EU reports mandate a 20% share of the gross energy consumption from renewable sources by 2020. Solar cells lead with a share increase of 15% in 2015, while energy savings are expected with more efficient lighting systems - illumination takes ca. 19% of the EU electrical energy. While current actions focus on developing either low-consumption lighting sources or efficient solar cells, DFID offers a game-changing vision with the ambitious aim to provide both targets into one dual-functional device that is a solar cell during the day and a lighting source during the night. The long-term scientific objective of DFID is to demonstrate how to control the intrinsic dual-functionality of ionic-based devices – lighting and photovoltaic – to elucidate their prospect. In particular, DFID’s strategy focuses on i) the establishment of basic knowledge about the device mechanism and ii) the design of novel sustainable materials, such as copper(I) coordination complexes and small-molecules.
Scientific highlights

Unveiling the dynamic processes in hybrid Lead Bromide Perovskite nanoparticle thin film devices

Perovskite (PK) materials are a promising next generation of semiconducting materials for thin film devices. Still the device mechanism is under hot debate since bulk PK films are both ionic and electronic conductors. Herein, long time poling schemes coupled to static and dynamic electrochemical impedance spectroscopy measurements allowed us to determine a dynamic device behavior related to the rearrangement of ionic species at the electrode interface ruling both charge injection and transport. Hence, this study opens up an alternative route toward understanding the dynamics inside hybrid perovskite materials based on the large body of knowledge of ionic-based optoelectronics.


Ultrafine nickel nanocatalyst-engineering layered double hydroxide towards high-efficiently fire-safe epoxy resin via interfacial catalysis

Multiscale design optimizes multi-functionality of nanomaterials as new generation of flame retardants [1-5]. Layered double hydroxide (LDH-DBS) nanosheets are surface-assembled by ultrafine Ni(OH)$_2$ nanocatalyst via the circular coordination-induced growth, aiming to achieve high-efficient fire safety of epoxy resin (EP). The design of LDH-DBS@Ni(OH)$_2$ is envisioned to exploit a spatial-dependent catalytic strategy to strengthening interfacial structure. Results illustrated that merely 3wt% LDH-DBS@Ni(OH)$_2$ imparted epoxy resin with UL-94 V-0 rating, accompanied by significant suppression of heat, smoke and carbon monoxide. Mechanism investigation by dynamic charring analysis revealed remarkable contribution of interfacial-charring catalysis to a reinforcement of intumescent char.

Figure 3. Schematic representation of the ionic-assisted dynamic behavior in perovskite-based devices.
Figure 4. Scheme 1 (a) Design and synthesis of LDH-DBS@Ni(OH)$_2$; (b) interfacial charring mechanism.

References:
programme

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.
Annual Report 2017

Design & Simulation of Composite Structures

High Performance Polymer Nanocomposites

Multifunctional Nanocomposites

Structural Composites

Nanomechanics

X-Ray Characterisation of Materials

The Next Generation of Composite Materials
Main research lines

Processing of high performance composites
- Optimisation of out-of-autoclave processing (injection/infusion/pultrusion or prepreg consolidation) and other manufacturing strategies including non-conventional curing strategies.

Recycling and repair of structural composites

New frontiers of structural performance
- Mechanical behaviour under low and high velocity impacts. Composites with non-conventional lay-up configuration. Hybrid composites.

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
- Simulation based smart manufacturing processes. Sensing and process control.
Projects in focus

ACERCOM / Fiber metal laminates for application in marine renewable energy

**Funding:** National Research Agency - Spanish Ministry of Economy and Competitiveness (MINECO). Collaboration Challenges 2016. (RTC-2016-5076-3)
**Partners:** Arcelor Mittal (Project Coordinator), Technical University of Madrid and IMDEA Materials Institute
**Project period:** 2016 – 2019
**Principal Investigator:** Prof. Carlos González

ACERCOM incorporate all the structural and functional requirements needed for the design of novel fiber metal laminates valid for application in marine renewable energies. Materials will be fully characterized with regards to their mechanical properties, resistance to extreme environments and fire behaviour. The conditions for industrial upscaling as machining, joining, conformability, etc. will be also analyzed within the project. In addition, simulation techniques for designing hybrid laminates accounting for the deformation and damage mechanisms in the metal and composite part will be developed. All these tools will be beneficial for the optimization of the material performances.

SIMUFORM / Interply friction behaviour in fresh composite laminates and implications in manufacturing

**Funding:** Fundación para la Investigación, Desarrollo y Aplicación de Materiales Compuesto (FIDAMC)
**Partners:** FIDMAC and IMDEA Materials Institute
**Project period:** 2017 – 2020
**Principal Investigator:** Prof. Carlos González

The main objective of the project is to develop physically based numerical methodologies based on finite elements to analyse and predict laminate deformation mechanisms occurring during fresh prepreg thermoforming. Traditionally, prepreg forming prior to curing was carried out manually or, for instance, by means of inflatable bladders. However, this procedure is costly and complex and is being replaced step-by-step by more automated systems based on hot presses. Moulding using hot presses is very effective but often leads to defects in the form of wrinkles and waviness due to the almost inextensible behaviour of carbon fibers. Predicting the occurrence of wrinkles is mandatory to produce the highest performance structural composites as well as lowering the cost associated with any tool modification.

**Figure 1.** Fiber metal laminate (steel and glass) manufactured by UPM subjected to three-point bending (courtesy of Prof. Suárez Bermejo).

**Figure 2.** FEM deformation pattern of a fiber metal laminate subjected to low velocity impact.

**Figure 3.** FEM deformation of a square fresh prepreg sheet during forming using and spherical indentor.
Scientific highlights

A Virtual Test Laboratory for composite laminates

The Composite Materials Programme has developed a reliable virtual testing framework for unidirectional laminated composites that allows the prediction of failure loads and modes of general in-plane coupons with great realism. This is a toolset based on finite element analysis that relies on a cohesive-frictional constitutive formulation coupled with the kinematics of penalty-based contact surfaces, on sophisticated three-dimensional continuum damage models, and overall on a modelling approach based on mesh structuring and crack-band erosion to capture the appropriate crack paths in unidirectional fibre reinforced plies. An extensive and rigorous validation of the overall approach was conducted, demonstrating that the virtual testing laboratory is robust and can be reliably used in for composite materials screening, design and certification.

Towards a comprehensive theory of void formation in liquid moulding manufacturing of composites

Out-of-autoclave manufacturing of composites by liquid moulding is nowadays a consolidated technique to produce composites with outstanding properties. However, during resin impregnation voids are formed as a consequence of the dual-scale porosity of the textiles. Flow occurs in a non homogeneous way, driven at the same time by capillary and viscous forces. If flow progresses slowly, voids are located in the yarn-to-yarn channels of the textile, while in the opposite case, voids are located inside the yarns at the microlevel. Thus, encompassing both types of flows will ensure that composites contain a minimum percentage of porosity. The Next Generation of Composite Materials program is collaborating with the Multiscale Characterization of Materials and Processes program to develop detailed experimental techniques based on X-ray tomography (fast tomography and laminography) to study in-situ void formation and transport mechanisms.
in real composite materials systems. These techniques are complemented with numerical simulations using fluid dynamics at the micro (tow) and meso level (ply) and jointly allow a complete optimization of the manufacturing parameters of the composite materials without the need for expensive experimental campaigns.

**Advanced sensors for manufacturing and health monitoring of composite materials**

Composite materials emerged several decades ago among the best candidates for lightweight structural applications, and in particular, for the aerospace sector. The assessment of the structural integrity of composites during service operations is mandatory and requires the need to continuously inspect structures to locate possible damaged areas as well as prepare the adequate inspection and prognosis campaigns. Fiber Bragg grating sensors, for instance, are mature techniques used for such purposes. However, these sensors are often embedded into the composite laminate producing remarkable distortions of the ply-by-ply structure as a consequence or their diameter. IMDEA Materials researchers are working together to find new sensors for composite materials based on the use of advanced CNT fibers. Such kind of CNT fibers are much less intrusive due to the smaller diameter size and can be adapted to the shape imposed by the laminate. In addition, CNT fibers can be used as sensors during impregnation and curing of the composite (Figure 9) and serve finally to control maximum deformations during service operations (Figure 10).

![Figure 7. a) Experimental set-up for XCT imaging during resin injection of composite materials, b) XCT tomogram showing voids entrapped in a plain woven composite.](image)

![Figure 8. Fluid dynamics simulation of the flow propagation process at the micro level including viscous and capillary forces.](image)

![Figure 9. Infusion test with embedded CNT fibers for flow front assessment.](image)

![Figure 10. Four point bending tests of a composite material laminate with embedded CNT fiber for strain analysis.](image)
programme

Novel Alloy Design, Processing and Development

Goal and vision

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 metallic alloys, with special emphasis on the role of microstructure on the mechanical response 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.
Main research lines

- **Characterisation** of microstructure and mechanical behaviour.

- **Advanced manufacturing:**
  - Solidification and casting.
  - Physical simulation of metallurgical processes (rolling, forging, extrusion, welding).

- **Additive manufacturing:**
  - Powder design and fabrication.
  - Process optimization.

- **Virtual processing:**
  Multi-scale modeling of solidification and phase transformations in metallurgical processing of metals and alloys.

- **Virtual testing:**
  Multi-scale modeling of the mechanical behavior of metallic polycrystals as function of their microstructure.

**Materials of Interest**

- **Metallic alloys for high temperature structural applications.** Ni/Co-based superalloys, NiAl, TiAl and FeAl alloys for aeroengine components.

- **Lightweight alloys and their composites.** For biomedical applications (Ti, Mg), electrical applications (Al alloys) or transport (Ti, Mg and nanocomposites).

- **High strength steels.** Quenched and partitioned steels with superior mechanical properties.
Projects in focus

**ALFORAMA / Innovative Al alloy for aircraft structural parts using Additive Manufacturing technology**

**Funding:** European Union, Horizon 2020 Programme (Grant Agreement 755610), Clean Sky Joint Undertaking 2

**Partners:** Lortek (Project Coordinator), University of Leuven and IMDEA Materials Institute

**Project period:** 2017 – 2020

**Principal Investigators:** Dr. Srdjan Milenkovic and Dr. Carmen Cepeda

The main goal of AlForAMA project is to develop an innovative High Strength Al alloy, feasible by powder metallurgy and suitable for Selective Laser Melting (SLM), with improved weldability and increased mechanical and corrosion resistance in comparison to cast grades Al alloys currently employed in Additive Manufacturing (AM). Selective Laser Melting (SLM), that utilizes a laser as a thermal energy source to melt the powder has been chosen as the preferred AM technology. Development of the innovative aluminium alloy specifically designed for SLM will be mainly focused on two different aspects: on one hand, on tailoring the chemical composition to improve processability and/or mechanical response of well-established commercial aluminium alloys and, on the other hand, on defining the SLM conditions to ensure a defect free material. Raw materials for SLM, produced in a powder form, will be obtained by casting and gas atomization. A suitable heat treatment will be optimized for the developed innovative Al alloy after its SLM processing.

**OptiQPAP / Optimization of quenched and partitioned steels designed for industrial applications**

**Funding:** European Union, Research for Coal and Steel (Grant Agreement 709755)

**Partners:** IMDEA Materials Institute (Coordinator), TATA steel, Thyssen Krupp Steel Europe AG, Centro Sviluppo Materiali, Fundació CTM Centre Tecnològic, TU Delft, Gent University

**Project period:** 2016 – 2019

**Principal Investigators:** Dr. Ilchat Sabirov

Advanced High Strength Steels processing via Quenching and Partitioning (Q&P) aims to produce steels containing martensite/retained austenite mixtures with desirable combination of strength, ductility and toughness. This project focuses on the intelligent microstructural design of high strength Q&P steels for the simultaneous improvement of different mechanical properties required for their commercialization. In particular attention is paid to fatigue and fracture behavior, wear resistance, weldability, ductile-brittle transition temperature, high strain rate behavior and energy absorption, along with the formability and bendability of Q&P steel.

**Figure 1. Aluminium powder produced by gas atomization.**

**Figure 2. Q&P Thermo-mechanical processing of a steel.**

**Figure 3. EBSD map of a steel after heat treatment.**
Scientific highlights

Unravelling the grain size effect on strength of polycrystalline alloys

It is well established that the strength of metallic alloys strongly depends on the grain size and phenomenological expressions as the Hall-Petch law are commonly used to consider this dependency. The physical origin of this effect has been studied by researchers of IMDEA Materials by means of a multiscale strategy based on finite element crystal plasticity simulation of the polycrystal. The mechanical behavior of each crystal is given by a dislocation-based crystal plasticity model that accounts for the dislocation storage at the grain boundaries. Polycrystalline copper is selected to validate the simulation strategy. The model is able to accurately predict the experimental results for a large range of grain sizes. It is found that the initial dislocation density plays a dominant role in the magnitude of the grain size effect and that dependence of flow stress with an inverse power of grain size (as predicted by Hall-Petch equation) breaks down for large initial dislocation densities and grain sizes.

Joining of dissimilar materials

The need of modern industry in low weight materials, their improved performance and functionality increases the use of hybrid structures, where the properties of different materials are jointly utilised to achieve best product performance. However, the joining process of dissimilar materials is a very challenging task due to significant difference of their properties. IMDEA Materials’ research activities in this area are two-fold: physical simulation of joining of dissimilar materials and advanced mechanical and microstructural characterization of the joints on macro- and micro-scales. Physical simulation of the joining process allows to reduce dramatically time and cost related with the development of novel routes for manufacturing of hybrid structures, as well as it enables the fundamental study of the effect of processing parameters on microstructure and properties of joints on different scales. Current research focuses on metal/metal and metal/composite joints and is carried out in collaboration with European and National partners, such as Université Catholique de Louvain and FIDAMC.

Additive Alloy Melting (ADAM) – A novel high-throughput casting method

The classical one-at-a-time research methodology to develop new materials limits technological progress. New strategies based on high-throughput (HT) techniques have been recently introduced to speed up materials innovation. However, most of the existing techniques are focused on thin films libraries, while methods for the generation of bulk materials are rather scarce. Researchers at IMDEA Materials have developed a novel method for accelerated alloy fabrication named additive alloy melting (ADAM). It is based on multiple sequential melting of several alloys in the arc melting furnace. Its effectiveness has been shown by modifying a commercial AISI 304 with 1-4 wt.% of Cu. In a single ingot, a range of compositions from 0 – 4 wt% Cu with a step of 1% were produced. XRF analysis showed that the corresponding spread of microstructures obtained matched the nominal compositions accurately with high level of homogeneity. Therefore, the developed method is unique in that i) it reduces the time required for the production of new alloys by casting several alloys with different composition in one single step and ii) it leaves a total freedom in the selection of the compositions to be cast.


Figure 6. Schematic of the method, ingots produced with their overall composition and homogeneity along the sample.
Integrated Computational Materials Engineering

Goal and vision

The research programme 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 programme 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 optimise materials for a given application (virtual design). Moreover, experiments are also an integral part of the research programme for the calibration and validation of the models at different length and time scales.

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

Computational Solid Mechanics

Modelling and Simulation of Materials Processing

Design & Simulation of Composite Structures

Mechanics of Materials

Computational and Data-Driven Materials Discovery
Main research lines

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

Projects in focus

**HYDTCOMP / Local hybridization of laminated composites for improved damage tolerance**

**Funding:** Spanish Ministry of Innovation and Competitiveness (National R&D Programme for Societal Challenges) (MAT2015-69491-C3-2-R)

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

**Project period:** 2016 – 2018

**Principal Investigators:** Dr. Cláudio S. Lopes and Dr. Juan José Vilatela

The fracture properties of composite materials can be improved by intelligently generating a heterogeneous microstructure. This can avoid “cascade” effects linked to the fact that the breaking of one fiber causes the break of adjacent ones, of very similar strength. These “cascade” or “avalanche” effects are largely responsible for the fragile behaviour of composites. 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 fiber composites. Increasing the energy dissipation in fracture events, expands the strain range at which it occurs and, therefore, reduces their brittleness, directly resulting in a weight reduction of the component. It is in this context that a stream of research emerged 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. With the help of advanced computational micromechanics, IMDEA Materials is studying the relevant micro-mechanisms and devising local hybridization approaches by mixing fibers within the same tow or ply.

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

**Funding:** European Union, Horizon 2020 Programme (Grant Agreement 669141). ERC Advanced grant

**Project period:** 2015 – 2020

**Principal Investigator:** Prof. Javier LLorca

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

*Figure 1. 3D Representative Volume Element (RVE) to study the process of fracture in hybrid composites.*
Scientific highlights

Multiscale modelling of precipitation strengthening in Al-Cu alloys
Towards bottom-up design strategies of metallic alloys

A multiscale modelling strategy has been developed to predict the homogeneous and heterogeneous nucleation of $\theta'$ (Al2Cu) precipitates in an Al-Cu alloy during high temperature aging. The model parameters that determine the different energy contributions (chemical free energy, interfacial energy, lattice parameters, elastic constants) were obtained from computational thermodynamics or first-principles density functional theory. From the information, the evolution and equilibrium morphology of the $\theta'$ precipitates is simulated in 3D using the phase-field model. The model was able to reproduce the evolution of the different orientation variants of plate-like shaped $\theta'$ precipitates with orientation relationship (001)$_\theta$//(001)$_\alpha$ and [100]$_\theta$//[100]$_\alpha$ during homogeneous nucleation as well as the heterogeneous nucleation on dislocations, leading to the formation of precipitate arrays (Fig. 2). Heterogeneous nucleation on pre-existing dislocations was triggered by the interaction energy between the dislocation stress field and the stress-free transformation strain associated to the nucleation of the $\theta'$ precipitates. Moreover, the mechanisms controlling the evolution of the morphology and the equilibrium aspect ratio of the precipitates were ascertained. All the predictions of the multiscale model were in good agreement with experimental data.

Once the precipitate structure has been obtained, the next step is to predict the hardening induced by their presence. This can be achieved by means of dislocation dynamics simulations in which a dislocation has to propagate through a forest of precipitates (Fig. 3). The lattice parameters, elastic constants and stress-free transformation strains of the precipitates were obtained by ab initio calculations while molecular dynamics simulations were used to determine the dislocation mobility, thus the multiscale simulations were parameter-free.

Figure 2. (a) Multiscale simulation of the nucleation and growth of $\theta'$ (Al2Cu) precipitates on dislocations during high temperature aging of an Al-Cu alloy. (b) Transmission electron microscopy micrograph showing the formation of a staircase structure of $\theta'$ precipitates on a dislocation. From H. Liu, B. Bellón, J. LLorca. Acta Materialia 132, 611-626, 2017.

Figure 3. Dislocation dynamics simulation of the propagation of a dislocation through a forest of $\theta'$ precipitates in an Al-Cu alloy.
Simulating the mechanical behaviour of polyurethane foams

In the framework of the EU project MODENA, a modelling strategy based on micromechanical characterization and computational homogenization was developed to determine the mechanical behaviour of rigid, closed-cell PU foams taking into account their microstructural features. The homogeneous macroscopic mechanical behaviour was numerically predicted by means of the finite element simulation of a representative volume element (RVE) of the PU foam. The foam microstructure in the model was obtained from the Laguerre tessellation of the space from a random close-packed distribution of spheres, which followed the measured foam cell size distribution. The geometric features of the foam cells were measured using X-ray computed tomography and the properties of the solid polyurethane in the foam were measured by means instrumented nanoindentation (Marvi et al., Int. J. Solids and Structures, 2018). This numerical tool reproduces very accurately the experimentally-observed behaviour of the foams up to large strains and captures well the effects of foam density, cell size distribution, cell anisotropy and others. Reliable surrogate models were then proposed as fast analytical tools to predict the behaviour of foams as function of these features.

Stable porous crystalline phases of molecular belts

The effort targets discovery of new porous molecular materials, which unlike framework porous materials, are rare. Porous molecular materials can sometimes be obtained by crystallization from a specially selected solvent, in which case they may lose their porosity upon solvent removal. By using an example of a molecular belt that shares this phenomenon, we demonstrated its structural modification that renders the molecule into a stable supramolecular nanotube porous crystal. Our approach involved computational crystal structure prediction and characterization as well as molecular dynamics simulations to determine stability of the predicted structures. (CrystEngComm 19, 6932, 2017)

Figure 4. Progressive simulation of the compressive behaviour of PU foams. The RVE approach is used to predict different stages of applied strain: elastic behaviour, plateau stress and foam densification.

Figure 5. Removal of methoxy groups from the macrocycle molecule on the left leads to the molecule on the right, which forms stable carbon nanotube analogue crystals.
programme

Multiscale Characterisation of Materials and Processes

Goal and vision

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.
Main research lines

3D characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques:

• X-Ray Tomography (XCT) and Diffraction (XRD).
• FIB-FEGSEM, including 3D-EDS, 3D-EDS and 3D-EBSD.
• TEM, including 3D-STEM and 3D-EDS.
• Correlative tomography studies, i.e., combining insights from different techniques.

4D characterisation: in-situ multiscale characterisation of processes:

• In-situ Mechanical testing across several length scales:
  - Tension, compression, fatigue, creep…of advanced metallic alloys and composites in the SEM and XCT.
  - Micro- and Nanomechanical Testing (nanoindentation, micropillar compression, microtensile testing…), including elevated temperature testing.
• In-situ characterisation of forming processes by XCT:
  - Infiltration and resin flow studies in composites.
  - Solidification studies.

Precipitates, growing along a dislocation line, in an Al-Cu alloy (3D-TEM).

Cross-correlation between experiments and multiscale simulations (ICME)
Projects in focus

**DYNACOMP / Dynamic behaviour of composite materials for next generation aeroengines**

*Funding:* European Union, Horizon 2020 Programme (Grant Agreement 722096). Marie Skłodowska-Curie-ITN-EID

*Academic partners:* IMDEA Materials Institute, (coordinator), Technical University of Madrid, Fundación Madri+d

*Industrial partners:* Hexcel Composites, Micromaterials Ltd.

*Project period:* 2016 – 2020

*Principal Investigators:* Dr. Jon Molina, Prof. Carlos González and Dr. Federico Sket

DYNACOM is a European Industrial Doctorate (EID) programme on the design of the next generation of structural composite materials for high strain rate applications. The main objective is the development of a consistent, physically based multiscale simulation strategy informed by the dynamic properties of the constituents (fiber, matrix and fiber/matrix interface) measured with a novel micromechanical testing methodology under impact conditions.

**EQUINOX / A novel process for manufacturing complex shaped Fe-Al intermetallic parts resistant to extreme environments**

*Funding:* European Union, Horizon 2020 Programme (Grant Agreement 689510). SC5

*Partners:* National Technical University, (coordinator), Elastotec GmbH Elastomertechniken, Dr. Kochanek Entwicklungsgesellschaft, IMDEA Materials Institute, Access e.V., Technical University of Liberec, OSM, FRENI BREMBO Spa, Yuzhnoye State Design Office, IRES.

*Project period:* 2016 – 2019

*Principal Investigators:* Dr. Srdjan Milenkovic and Dr. Federico Sket

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 with a novel near net shape production technology for a new class of highly advanced ductile Fe-Al based intermetallics. For this purpose Fe porous preforms are processed via reactive-infiltration with Al or Al-alloys.

*Figure 1.* Composite fan blades on a GE GEnx-2B engine (www.compositesworld.com).

*Figure 2.* Micromechanical tests to apply at impact conditions: (a) Indentations made on a cross-section of a CFRP. (b) pushed-out debonded fiber.

*Figure 3.* Porous iron preforms used for Al and Al alloy melt infiltration (a) XCT volume of SLM sample. (b) porosity evaluation of the respective preforms.
Scientific highlights

**Slip transfer across \(\gamma\)-TiAl lamellae in tension**

Gamma (\(\gamma\)) TiAl based alloys have very attractive specific properties that make them crucial to meet the requirements of the next generation of aircraft engines. The main drawback, however, is their limited ductility, caused partly by the complex lamellar microstructure. This work identifies the mechanisms governing dislocation transmission across lamellar interfaces in a Ti-45Al-2Nb-2Mn (at.%) + 0.8 (vol%) TiB\(_2\) (Ti4522XD) alloy, by combining in-situ microtensile testing, EBSD and TEM.

**Effect of processing parameters on the reaction kinetics of Fe-Al intermetallics by combined radiography and diffraction**

The effect of processing parameters on the kinetics of solidification and formation of Fe-Al intermetallic phases is an unknown subject in materials science. In this experiment we look inside the reactive infiltration process with two sets of “eyes”: X-ray radiography (XR) and X-ray diffraction (XRD). For that, we have developed an in-situ infiltration device that allows us to follow not only the melt flow mechanisms but also the reaction velocity and reaction front between molten Al and solid Fe.


Figure 4. (a) Scheme of the experiment set up at a synchrotron beamline. (b) XCT of the reacted preform after infiltration. (c) EBSD map of the same reacted preform showing the different phases formed during reactive infiltration.
Fatigue crack initiation and propagation studies in Ni superalloys

The fatigue growth of microstructural short cracks is an area that remains relatively unexplored. Thus, the development of novel experimental tests to develop a better understanding of the mechanisms involved in the nucleation and propagation of short cracks is crucial, especially to develop predictive multiscale models of fatigue. For this, in-situ High Cycle Fatigue (HCF) tests were carried out at beamline ID11 at ESRF, in Inconel 718 test specimens. Diffraction Contrast Tomography (DCT) was initially performed to reveal the 3D grain structure of each specimen and Phase Contrast Tomographs (PCT) were acquired at regular intervals using white beam radiation, to study the evolution of crack nucleation and propagation with the number of fatigue cycles.

The combination of both, DCT and PCT techniques, allows tracking of the crack path through the interior of the sample, thus leading to an exhaustive 3D study of that path as a function of grain misorientation.

Figure 5. (a) Scheme of the experiment set up at a synchrotron beamline. (b) Initial grain structure by DCT in the gauge length and (c) Crack evolution with number of fatigue cycles determined by PCT.
strategic emerging technologies

As part of the continuous strategy of IMDEA Materials Institute, the research programmes have identified three emerging technologies of high industrial and scientific relevance. During 2017 the Institute has invested internal resources, in collaboration with other research institutions and companies, for the development of these ambitious technologies which will enable product and process innovations in different sectors.
Towards fire-safe structural batteries

Goals
Development of new battery concepts combining: high efficiency, light-weight, augmented mechanical properties (structural, toughness) and improved fire-safety.

Strategy
Combination of expertise of different research groups in molecular design, synthesis of advanced nanostructured current collectors and active materials, development of fire-retardants and polymer electrolytes, device fabrication and in-situ characterisation, and multi-physics study of laminated structures and devices.

---

Figure 1. Scheme of a battery operation.

Figure 2. 3D X-ray tomography of an energy-storing structural composite.

Figure 3. Simulation of the deformation of an energy-storing laminated structure.
**Damage-tolerant additive manufacturing of metallic alloys**

**Goals**
Development of novel additive manufacturing (AM) strategies for metallic alloys that combines the benefits of this processing route with a damage-tolerant behaviour.

**Strategy**
Combination of expertise of different research groups in design and fabrication of metallic powders, process monitoring, multi-physics modelling of AM, multiscale modelling of solidification and high throughput characterisation techniques.

*Figure 4. Selective Laser Melting (SLM) system.*

*Figure 5. Arc melting furnace and gas atomiser.*

*Figure 6. Multiscale modelling strategy of SLM processing.*
Simulation-based smart manufacturing of composites

Goals
Development of smart manufacturing strategies to automatically detect and recognize processing disturbances occurring during composite manufacturing by means of resin injection and infusion. Signals acquired using sensor network will help to detect failure patterns and decide the appropriate corrective actions in order to reduce costs and part rejection during manufacturing.

Strategy
Use machine learning algorithms in combination with multiphysics simulations to help to detect processing disturbance patterns occurring during manufacturing. Algorithms are trained using experimental results acquired with advanced in-situ sensoring as well as synthetic data generated from fluid flow simulations.

Figure 7. Sketch of a typical resin injection process RTM. Resin inhomogeneous flow is produced as a consequence of manufacturing disturbances that induce the formation of defect in the composite part.

Figure 8. Flow front in a resin infusion process.

Figure 9. Detail of a stringer-skin integration manufactured by resin transfer moulding RTM.
principal investigators
Senior Researchers

Prof. Ignacio Romero
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. María Teresa Pérez-Prado
Deputy Director, 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; design of novel alloys for additive manufacturing; in situ investigation of the deformation and recrystallization mechanisms of light and high temperature metals; fabrication of novel metallic phases with improved mechanical and functional properties by non-equilibrium processing.
Prof. Javier LLorca  
Scientific 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 modelling 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 processing-microstructure-properties relationships in advanced structural materials.

Prof. Carlos González  
Senior Researcher, Structural Composites  
Ph.D. in Materials Science from Technical University of Madrid. Spain  
Professor of Materials Science, Technical University of Madrid  

Research Interests  
Materials processing, characterisation and modelling from a theoretical and numerical perspective of the mechanical performance of advanced structural materials with special emphasis in polymeric-matrix composites; development of physically-based constitutive models including multiscale strategies for virtual testing as well as virtual processing for manufacturing optimization.

Dr. Jon M. Molina-Aldareguía  
Senior Researcher, Micromechanics and Nanomechanics  
Ph.D. in Materials Engineering from Cambridge University. United Kingdom  

Research Interests  
Micro- and nano-mechanical testing and advanced focused-ion beam and electron microscopy analysis of advanced structural materials; microstructural and mechanical characterisation of thin-films; mechanical testing inside the scanning and transmission electron microscopes.
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. Cláudio 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 materials and structures; multiscale computational analysis of composites; damage and failure of composite materials; impact and damage tolerance of composite structures; non-conventional multiscale composite design and manufacturing; additive manufacturing of composites; recycling of composite materials.

Dr. Juan José Vilatela
Senior Researcher, Multifunctional Nanocomposites
Ph.D. in Materials Science from University of Cambridge, United Kingdom

Research Interests
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. Study of their hierarchical structures by advanced X-ray techniques, reinforcement at multiple lengthscales 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 and harvest 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 nanostructure materials, design and processing of high performance polymers and their nanocomposites, with particular emphasis in structural properties and behaviour under fire.
Dr. Srdjan Milenkovic
Senior Researcher, Solidification Processing & Engineering
Ph.D. in Materials Engineering from State University of Campinas, Brazil

Research Interests
Advanced solidification processing techniques (centrifugal and suction casting, reactive infiltration) with special emphasis on small scale gas atomization of powders for additive manufacturing and development of novel high-throughput casting methods for accelerated material discovery by means of materials libraries. Alloy development, processing-structure-property relationships of Ni-based superalloys, intermetallic compounds eutectic alloys and other advanced materials for high-temperature applications.

Dr. Ilchat Sabirov
Senior Researcher, Physical Simulation
Ph.D. in Metallurgy from Montanuniversitaet Leoben, Austria

Research Interests

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. Novel methodologies that effectively combine materials informatics approaches with computational material science techniques such as electronic structure calculations and/or molecular simulations. The developed methodologies are verified and/or integrated with experiments conducted in collaborating groups. Their applications are broad but can be collectively described as the design of materials for clean and energy efficient technologies.

Dr. Ruben D. Costa
Senior Researcher, Hybrid Optoelectronic Materials and Devices
Ph.D. in Chemistry from the University of Valencia, Spain

Research Interests
Research going from the design and preparation of new materials to the fabrication and optimization of devices for lighting and energy conversion applications. This is rounded by a full-fledged expertise in electrochemical, photophysical, and theoretical techniques. The goal is to progress the technologies above fulfilling the “green photonics” concept. His research encompasses three lines: i) hybrid organic-inorganic materials for solar harvesting and lighting purposes, ii) 3rd generation of electroactive materials for electroluminescent paints, and iii) biomaterials for lighting and photovoltaics.
Researchers

**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.

**Dr. Vinodkumar Etacheri**
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. Damien Tourret**
Researcher, Modelling and Simulation of Materials Processing
Ph.D. in Materials Science and Engineering from Mines ParisTech, France

**Research Interests**
Microstructure selection, formation, and evolution; solidification processing (e.g. casting, welding, additive manufacturing); structural materials; metals and alloys; crystal growth; phase transformations; multiscale modelling; phase-field modelling; parallel computing (e.g. using graphics processing units); nonequilibrium solidification; directional solidification experiments; in situ imaging of metals and alloys.
Visiting Scientists

**Prof. Mauricio Terrones**  
Visiting Scientist, Low Dimensional Materials  
Ph.D. in Chemical Physics from the University of Sussex.  
United Kingdom  
Distinguished Professor of Physics, Chemistry and Materials Science & Engineering, Penn State University. USA  

Research Interests  
The study of low dimensional materials that mainly involve one-two dimensions, ranging from carbon nanotubes and graphene nanoribbons to graphene, boron nitride and chalcogenide monolayers (e.g. WS$_2$, MoS$_2$, NbS$_2$, etc). In particular, the challenging synthesis of novel nanoscale materials (1D and 2D) with unprecedented physico-chemical properties. We also explore possible applications of these materials, including molecular sensors, photo-detectors, multifunctional coatings, virus detection/isolation, and batteries.

**Dr. Roberto Guzmán de Villoria**  
Visiting Scientist, Nano-Architectures and Materials Design  
Ph.D. in Mechanical Engineering from the University of Zaragoza. Spain  

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

**Prof. Thomas Bieler**  
Visiting Scientist, Physical Metallurgy, Grain Boundaries and Crystal Plasticity  
Ph.D. in Materials Science from the University of California. United States of America  
Professor of Materials Science, Michigan State University. USA  

Research Interests  
Characterization of mesoscale deformation mechanisms and plasticity modeling in titanium based alloys, tin (lead-free solder joints), and high purity niobium used in superconducting particle accelerator cavities.

**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 semibiocomposites or biocomposites based on starch and lignin.

**Dr. Yuwen Cui**  
Visiting Scientist, Computational Alloy Design  
Ph.D. in Materials Science from Central South University. China  
Professor of Materials Science, Nanjing Tech 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.
## annex

<table>
<thead>
<tr>
<th>Topic</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>R&amp;D projects and contracts</td>
<td>63</td>
</tr>
<tr>
<td>fellowships</td>
<td>72</td>
</tr>
<tr>
<td>scientific results</td>
<td>80</td>
</tr>
<tr>
<td>training and dissemination activities</td>
<td>105</td>
</tr>
</tbody>
</table>
1. R&D Projects and Contracts

1.1. International R&D Projects

Title/Acronym: Innovative Al alloy for aircraft structural parts using Additive Manufacturing technology/ALFORAMA
Partners: IK4-Lortek (Coordinator), University of Leuven, IMDEA Materials Institute
Period: 2017 – 2020
Funding Institution/Programme: European Union/Horizon 2020 Programme – Clean Sky Joint Undertaking 2
Principal Investigators: Dr. Srdjan Milenkovic and Dr. Carmen Cepeda

Title/Acronym: Structural power composites for future civil aircraft/SORCERER
Partners: Imperial College (Coordinator), Chalmers University of Technology, KTH Royal Institute of Technology, IMDEA Materials Institute
Period: 2017 – 2020
Funding Institution/Programme: European Union/Horizon 2020 Programme – Clean Sky Joint Undertaking 2
Principal Investigator: Dr. Juan José Vilatela

Title/Acronym: New approach to manufacturing of advanced nanostructured Al-based conductors with enhanced mechanical and functional properties/ALCON
Partners: Saint-Petersburg State University, IMDEA Materials Institute
Period: 2017 – 2019
Funding Institution/Program: Ministry of Education and Science of the Russian Federation
Principal Investigator: Dr. Ilchat Sabirov

Title/Acronym: Tailored metal-organic framework: from hybrid to multifunctional flame retardant polymer nanocomposites/MOFMAP
Partners: IMDEA Materials Institute
Period: 2017 – 2019
Funding Institution/Programme: European Union/Horizon 2020 Programme – Marie Skłodowska-Curie actions - IF
Principal Investigator: Dr. Xiao-Lin Qi
Supervisor: Dr. De-Yi Wang

Title/Acronym: Structural energy harvesting composite materials/STEM
Partners: IMDEA Materials Institute
Period: 2016 – 2021
Funding Institution/Programme: European Union/Horizon 2020 Programme – ERC Starting Grant
Principal Investigator: Dr. Juan José Vilatela
Title/Acronym: CROR engine debris impact shielding. Design, manufacturing, simulation and impact test preparation/REDISH  
Partners: IMDEA Materials Institute (Coordinator), Foundation for Research Development and Application of Composite Materials (FIDAMC)  
Period: 2016 – 2018  
Funding Institution/Programme: European Union/Horizon 2020 Programme – Clean Sky Joint Undertaking 2  
Principal Investigator: Dr. Cláudio S. Lopes

Title/Acronym: Optimization of quenched and partitioned steels designed for industrial applications/OPTIQPAP  
Partners: IMDEA Materials Institute (Coordinator), Fundació CTM Centre Tecnològic, ThyssenKrupp Steel Europe AG, University of Gent, Centro Sviluppo Materiali, Technical University of Delft, TATA Steel Nederland Technology  
Period: 2016 – 2019  
Funding Institution/Programme: European Union/Research Fund for Coal and Steel  
Principal Investigator: Dr. Ilchat Sabirov

Title/Acronym: A novel process for manufacturing complex shaped Fe-Al intermetallic parts resistant to extreme environments/EQUINOX  
Period: 2016 – 2019  
Funding Institution/Programme: European Union/Horizon 2020 Programme – SC5  
Principal Investigators: Dr. Srdjan Milenkovic y Dr. Federico Sket

Title/Acronym: Dynamic behaviour of composite materials for next generation aeroengines/DYNACOMP  
Partners: IMDEA Materials Institute (Coordinator), HEXCEL Composites, Micro Materials Ltd., Technical University of Madrid, Madri+d foundation  
Period: 2016 – 2020  
Funding Institution/Programme: European Union/Horizon 2020 Programme – Marie Skłodowska-Curie actions - ITN - EID  
Principal Investigators: Dr. Jon M. Molina, Prof. Carlos González and Dr. Federico Sket
Title/Acronym: Multi-functional nano-carbon composite materials network/MULTICOMP  
Partners: Multiple partners coordinated by the Karlsruhe Institute of Technology (Coordinator)  
Period: 2016 – 2020  
Funding Institution/Programme: European Union/Horizon 2020 Programme – COST Actions  
Principal Investigator: Dr. Juan Pedro Fernández

Title/Acronym: Virtual design, processing and testing of advanced metallic alloys for engineering applications/VIRMETAL  
Partners: IMDEA Materials Institute  
Period: 2015 – 2020  
Funding Institution/Programme: European Union/Horizon 2020 Programme – ERC Advanced Grant  
Principal Investigator: Prof. Javier LLorca

Title/Acronym: Pilot manufacturing line for production of highly innovative materials/PILOTMANU  
Partners: MBN Nanomaterialia (Coordinator), +90, Putzier, INOP, Manudirect, Centre for Process Innovation, IMPACT INNOVATIONS GmbH, Matres, Diam Edil SA, IMDEA Materials Institute  
Period: 2013 – 2017  
Funding Institution/Programme: European Union/7th Framework Programme - NMP  
Principal Investigator: Dr. Andrea García-Junceda

1.2. National R&D Projects

Title/Acronym: The high temperature fatigue behavior of a third generation gamma TiAl alloy for greener turbines/CRACK-TIAL  
Partners: IMDEA Materials Institute  
Period: 2017 – 2019  
Principal Investigators: Dr. Teresa Perez-Prado and Dr. Ilchat Sabirov
Title/Acronym: Ultrafine eutectics by laser additive manufacturing/ELAM  
Partners: German Aerospace Research Center (Coordinator), Access e.V., Wigner Research Centre for Physics, Fraunhofer Institute for Laser Technology, Bosch-Mahle Turbosystems GmbH, P&G Manufacturing GmbH, IMDEA Materials Institute  
Period: 2017 – 2020  
Principal Investigator: Dr. Federico Sket

Title/Acronym: Fiber metal laminates for application in marine renewable energy/ACERCOM  
Partners: ArcelorMittal (Coordinator), Technical University of Madrid, IMDEA Materials Institute  
Period: 2016 – 2019  
Principal Investigator: Prof. Carlos González

Title/Acronym: Advanced materials and nanomaterials Spanish technological platform/MATERPLAT  
Partners: IMDEA Materials Institute (Technical Secretariat)  
Period: 2016 – 2018  
Platform Coordinator: Miguel Ángel Rodiel

Title/Acronym: Intralaminar hybridization, use of scraps and analysis of their effects. Characterization and modeling/HYDTCOMP  
Partners: University of Girona (Coordinator), IMDEA Materials Institute  
Period: 2016 – 2018  
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges 2015  
Principal Investigators: Dr. Cláudio S. Lopes and Dr. Juan José Vilatela
Title/Acronym: Multiscale approach for the simulation of thermomechanical problems under severe conditions: application to machining/EMULATE
Partners: IMDEA Materials Institute (Coordinator) Mondragón University, Technical University of Madrid
Period: 2016 – 2018
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges 2015
Principal Investigator: Prof. Ignacio Romero

Title/Acronym: Innovative additives for foams with improved thermal insulation and fire resistance/NEOADFOAM
Partners: TOLSA S.A. (Coordinator), University of Valladolid, IMDEA Materials Institute
Period: 2015 – 2018
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness (MINECO)/ National Programme of Research, Development and Innovation Oriented Challenges of the Society. Collaboration Challenges 2015
Principal Investigator: Dr. De-Yi Wang

Title/Acronym: Development of computational and experimental techniques for analysis and design of fire retardant polymers/COMETAD
Partners: International Center for Numerical Methods in Engineering (CIMNE) (Coordinator), IMDEA Materials Institute
Period: 2015 – 2017
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges 2014
Principal Investigator: Dr. De-Yi Wang
Title/Acronym: Study of sepiolite-based fire retardant systems/SEPIFIRE
Partners: TOLSA S.A. (Coordinator), Materials Science Institute of Madrid (ICMM-CSIC), IMDEA Materials Institute
Period: 2014 – 2017
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Collaboration Challenges 2014
Principal Investigator: Dr. De-Yi Wang

1.3. Regional R&D Projects

Title/Acronym: Dual-functional ionic-based devices: electroluminescence and photovoltaic responses in one
Partners: IMDEA Materials Institute
Period: 2017 – 2021
Funding Institution/Programme: Madrid Regional Government/Grant for research talent attraction. Modality 1
Principal Investigator: Dr. Ruben D. Costa

Title/Acronym: The next generation of rechargeable Li-O₂ batteries
Partners: IMDEA Materials Institute
Period: 2017 – 2021
Funding Institution/Programme: Madrid Regional Government/Grant for research talent attraction. Modality 1
Principal Investigator: Dr. Vinodkumar Etacheri

Title/Acronym: Experimental characterization and analysis of grain boundary sliding with anisotropic cohesive zone modeling in a crystal plasticity finite element microstructure model environment
Partners: IMDEA Materials Institute
Period: 2017 – 2018
Funding Institution/Programme: Madrid Regional Government/Grant for research talent attraction. Modality 3
Principal Investigator: Prof. Thomas Bieler

Title/Acronym: Establishment of a scientific platform of two-dimensional (2D) layer-by-layer materials applicable to “foldable” electronic structures
Partners: IMDEA Materials Institute
Period: 2017 – 2018
Funding Institution/Programme: Madrid Regional Government/Grant for research talent attraction. Modality 3
Principal Investigator: Prof. Mauricio Terrones
### Title/Acronym: Multiscale design of advanced materials/DIMMAT
**Partners:** IMDEA Materials Institute (Coordinator), National Centre of Metallurgical Research (CENIM-CSIC), Carlos III University of Madrid, Complutense University of Madrid, Materials Science Institute of Madrid (ICMM-CSIC), Technical University of Madrid
**Period:** 2014 – 2018
**Funding Institution/Programme:** Madrid Regional Government/Programme of R&D activities between research groups in Technology
**Principal Investigator:** Dr. Teresa Perez-Prado

### Title/Acronym: Fundamental properties and applications of graphene and other bidimensional materials/MAD2D
**Partners:** IMDEA Nanoscience Institute (Coordinator), Materials Science Institute of Madrid (ICMM-CSIC), IMDEA Materials Institute, IMDEA Energy Institute, Autonomous University of Madrid
**Period:** 2014 – 2018
**Funding Institution/Programme:** Madrid Regional Government/Programme of R&D activities between research groups in Technology
**Principal Investigator:** Dr. Juan José Vilatela

### 1.4. Privately-funded R&D Projects

#### Title/Acronym: Microstructure based material mechanical model for superalloys/MICROMECH II
**Company:** ITP Aero
**Period:** 2017 – 2019
**Principal Investigator:** Dr. Javier Segurado

#### Title/Acronym: Study of the comprehensive utilization Magnesium sources in the salt lakes/SUMER
**Institution:** Qinghai Institute of Salt Lakes
**Period:** 2017 – 2019
**Principal Investigator:** Dr. De-Yi Wang

#### Title/Acronym: New, innovative halogen-free flame retardant products/INNOFLAME
**Company:** Archroma Management GmbH
**Period:** 2017
**Principal Investigator:** Dr. De-Yi Wang
Title/Acronym: Physical simulation of heat treatment of coated steel specimens using Gleeble system  
Company: ArcelorMittal Spain  
Period: 2017  
Principal Investigator: Dr. Ilchat Sabirov

Title/Acronym: New material solutions for the optimization of AC roof units/MAVIS  
Company: Sanz Clima  
Period: 2017 – 2018  
Principal Investigator: Dr. De-Yi Wang

Title/Acronym: Data dispersion study in IN718 and ballistic tests in TiAl/ IMPACT TiAl  
Company: ITP Aero  
Period: 2017 – 2018  
Principal Investigators: Dr. Jon M. Molina and Dr. Ilchat Sabirov

Title/Acronym: New fire retardant additives to polymers/NEWTOP  
Company: Liaoning Jinghua New Materials Inc.  
Period: 2017 – 2018  
Principal Investigator: Dr. De-Yi Wang

Title/Acronym: Study of the mechanisms of actuation of polyols with fire retardant capabilities /FIREMEC  
Company: Repsol S.A.  
Period: 2017 – 2018  
Principal Investigator: Dr. De-Yi Wang

Title/Acronym: Interply friction behaviour in fresh composite laminates and implications in manufacturing/SIMUFORM  
Institution: Foundation for the research development and application of composite materials (FIDAMC)  
Partners: IMDEA Materials Institute (coordinator) and Foundation for the research development and application of composite materials (FIDAMC)  
Period: 2017 – 2019  
Principal Investigator: Prof. Carlos González

Title/Acronym: Front fuselage crashworthiness modelling/CRASHING II  
Company: AIRBUS Defence & Space  
Period: 2016 – 2017  
Principal Investigator: Dr. Cláudio S. Lopes
<table>
<thead>
<tr>
<th>Title/Acronym</th>
<th>Company</th>
<th>Period</th>
<th>Principal Investigators</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modular concept for ultralight removable advanced car seat/ADVANSEAT</td>
<td>Grupo Antolín</td>
<td>2015 – 2018</td>
<td>Prof. Carlos González and Dr. Cláudio S. Lopes</td>
</tr>
<tr>
<td>Development of new structural materials for energy harvesting and storage/DESMAN</td>
<td>B/E AEROSPACE</td>
<td>2014 – 2017</td>
<td>Dr. Juan José Vilatela</td>
</tr>
<tr>
<td>Development and validation of simulation methods for ice and bird ingestion in plane engines/SIMUFOING</td>
<td>ITP Aero</td>
<td>2014 – 2017</td>
<td>Prof. Ignacio Romero</td>
</tr>
<tr>
<td>Multiscale virtual testing of CFRP samples/VIRTEST</td>
<td>Fokker Aerostructures B.V.</td>
<td>2014 – 2018</td>
<td>Dr. Cláudio S. Lopes</td>
</tr>
<tr>
<td>Online NDT RTM inspection in composites/ONLINE RTM</td>
<td>AIRBUS Operations S.L.</td>
<td>2014 – 2018</td>
<td>Prof. Carlos González</td>
</tr>
<tr>
<td>A study of the factors influencing air removal in out-of-autoclave processing of composites/AROOA</td>
<td>HEXCEL Composites</td>
<td>2014 – 2017</td>
<td>Dr. Federico Sket and Prof. Carlos González</td>
</tr>
<tr>
<td>Structural analysis of the iter pre-compression rings/ITER PCRs</td>
<td>AIRBUS Defence &amp; Space</td>
<td>2012 – 2018</td>
<td>Prof. Carlos González</td>
</tr>
</tbody>
</table>
2. Fellowships

2.1. International

Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Period: 2017
Funding Institution: European Union
Dr. D. Tourret

Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Period: 2017
Funding Institution: European Union
Dr. S. Hu

Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Period: 2016-2017
Funding Institution: European Union
Dr. W. Li

Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Period: 2016-2017
Funding Institution: European Union
Dr. A. Moitra

Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Period: 2016-2017
Funding Institution: European Union
Dr. S. Djaziri

Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Period: 2016-2017
Funding Institution: European Union
Dr. S. Haouala
Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Period: 2016-2017
Funding Institution: European Union
Dr. X. Wen

Programme: AMAROUT EUROPE II, Marie Curie Action (PEOPLE-COFUND), 7th Framework Programme
Funding Institution: European Union
Dr. V. B. Heeralal

Programme: China Scholarship Council fellowships
Project: Magnesium alloys
Period: 2017-2021
Funding Institution: China Scholarship Council
D. Shi

Programme: China Scholarship Council fellowships
Project: New carbon based polymer composites
Period: 2017-2019
Funding Institution: China Scholarship Council
W. Qi

Programme: China Scholarship Council fellowships
Project: Energy storage, batteries, nanomaterials
Period: 2017-2021
Funding Institution: China Scholarship Council
W. Fen

Programme: China Scholarship Council fellowships
Project: Eco-friendly fire retardant coating
Period: 2016-2019
Funding Institution: China Scholarship Council
C. Fu

Programme: China Scholarship Council fellowships
Project: Multi-functional graphene thermoplastic composite materials
Period: 2016-2020
Funding Institution: China Scholarship Council
Y. Ou
Programme: China Scholarship Council fellowships
Project: High strain rate mechanical behavior of advanced high strength steels
Period: 2016-2020
Funding Institution: China Scholarship Council
X. Peikang

Programme: China Scholarship Council fellowships
Project: Multifunctional fire retardant for polymer
Period: 2016-2020
Funding Institution: China Scholarship Council
J. Zhang

Programme: China Scholarship Council fellowships
Project: Development of innovative materials for the cutting tools industry
Period: 2015-2018
Funding Institution: China Scholarship Council
X. Deng

Programme: China Scholarship Council fellowships
Project: Numerical models for thermo-mechanically coupled crystal plasticity
Period: 2015-2019
Funding Institution: China Scholarship Council
J. Li

Programme: China Scholarship Council fellowships
Project: Kinetics of magnesium alloys
Period: 2015-2019
Funding Institution: China Scholarship Council
N. Li
Programme: China Scholarship Council fellowships  
Project: Computational thermodynamics of Magnesium alloys  
Period: 2015-2019  
Funding Institution: China Scholarship Council  
J. Wang

Programme: China Scholarship Council fellowships  
Project: Polymer composites and nanocomposites  
Period: 2015-2019  
Funding Institution: China Scholarship Council  
L. Zhang

Programme: China Scholarship Council fellowships  
Project: High throughput diffusion and phase transformation  
Period: 2014-2018  
Funding Institution: China Scholarship Council  
C. Wang

Programme: China Scholarship Council fellowships  
Project: Fire retardant polymeric materials  
Period: 2013-2018  
Funding Institution: China Scholarship Council  
Y. Pan

Programme: China Scholarship Council fellowships  
Project: Nanoscale metal-ceramic multilayers  
Period: 2013-2018  
Funding Institution: China Scholarship Council  
L. Yang

Programme: China Scholarship Council fellowships  
Project: High performance environmentally friendly fire retardant epoxy nanocomposites  
Period: 2012-2017  
Funding Institution: China Scholarship Council  
X. Zhao

Programme: Doutorado Sanduíche  
Project: Hypoeutectic Zn-Al alloys by powder metallurgy  
Period: 2017-2018  
Funding Institution: CAPES Foundation, Brazil  
K. Kazmierczak
2.2. National

Programme: *Ramon y Cajal*
Period: 2015-2020
Funding Institution: *Spanish Ministry of Economy and Competitiveness*
Dr. M. Haranczyk

Programme: *Ramon y Cajal*
Period: 2015-2020
Funding Institution: *Spanish Ministry of Economy and Competitiveness*
Dr. J. J. Vilatela

Programme: *Ramon y Cajal*
Period: 2013-2018
Funding Institution: *Spanish Ministry of Economy and Competitiveness*
Dr. C. Lopes

Programme: *Postdoctoral Fellowship*
Period: 2017-2019
Funding Institution: *Spanish Ministry of Economy and Competitiveness*
Dr. D. Wang

Programme: *Postdoctoral Fellowship*
Period: 2017-2019
Funding Institution: *Spanish Ministry of Economy and Competitiveness*
Dr. A. Baluch

Programme: *Training University Lecturers (FPU)*
Period: 2017-2021
Funding Institution: *Spanish Ministry of Education, Culture and Sport*
A. Fernández

Program: *Training University Lecturers (FPU)*
Period: 2016-2020
Funding Institution: *Spanish Ministry of Education, Culture and Sport*
B. Bellón
Program: Training University Lecturers (FPU)
Period: 2015-2017
Funding Institution: Spanish Ministry of Education, Culture and Sport
L. C. Herrera

Programme: Predoctoral Fellowships
Period: 2017-2020
Funding Institution: Spanish Ministry of Economy and Competitiveness
M. Barzegar

Programme: Predoctoral Fellowships
Period: 2013-2017
Funding Institution: Spanish Ministry of Economy and Competitiveness
A. Palomares

Programme: Youth Employment Programme
Period: 2015-2017
Funding Institution: Spanish Ministry of Economy and Competitiveness
C. Andradas

Programme: Youth Employment Programme
Period: 2015-2017
Funding Institution: Spanish Ministry of Economy and Competitiveness
J. Castro

Programme: Youth Employment Programme
Period: 2015-2017
Funding Institution: Spanish Ministry of Economy and Competitiveness
M. Cejuela
Programme: Youth Employment Programme  
Period: 2015-2017  
Funding Institution: Spanish Ministry of Economy and Competitiveness  
H. Mora

---

2.3. Regional

Programme: Talent Atraction Programme – Modality 2  
Period: 2017-2021  
Funding Institution: Spanish Ministry of Economy and Competitiveness  
Dr. Z. Liu

Programme: Youth Employment Programme / Research assistants and laboratory technicians  
Period: 2017-2019  
Funding Institution: Madrid Regional Government  
A. Doñoro

Programme: Youth Employment Programme / Research assistants and laboratory technicians  
Period: 2017-2019  
Funding Institution: Madrid Regional Government  
A. Larrañaga

Programme: Youth Employment Programme / Research assistants and laboratory technicians  
Period: 2017-2019  
Funding Institution: Madrid Regional Government  
J. de la Vega

Programme: Youth Employment Programme / Research assistants and laboratory technicians  
Period: 2017-2019  
Funding Institution: Madrid Regional Government  
A. Martín

Programme: Youth Employment Programme / Research assistants and laboratory technicians  
Period: 2016-2018  
Funding Institution: Madrid Regional Government  
F. Fernández
Programme: Youth Employment Programme / Research assistants and laboratory technicians
Period: 2016-2017
Funding Institution: Madrid Regional Government
N. Pérez

Programme: Youth Employment Programme / Predoctoral researchers
Period: 2017-2018
Funding Institution: Madrid Regional Government
S. Lucarini

Programme: Youth Employment Programme / Predoctoral researchers
Period: 2017-2018
Funding Institution: Madrid Regional Government
C. Gutierrez
3. Scientific Results

3.1. Publications


57. B. Alemán, R. Ranchal, V. Reguero, B. Mas, and J. J. Vilatela. Carbon nanotube fibers with martensite and austenite Fe residual catalyst: room temperature


### 3.3. Book Chapters


### 3.4. Patent Applications


3.5. International Conferences

Invited and Plenary talks


Regular Contributions


30. “Modeling of fatigue fracture of Inconel 718 by means of crystal plastic and computational homogenization”, J. Segurado, A. Cruzado, S. Lucarini, J. LLorca,


Membership in Organising Committees


### 3.6. Hosting and Organisation of International Conferences and Workshops


3.7. Invited Seminars and Lectures

12. “A roadmap for virtual design of metallic materials: from atoms to components”, J. LLorca, Department of Mechanical Engineering, Purdue University, West Lafayette, Indiana, USA, May 2017.
17. “Computational metallurgy (Métallurgie numérique)”, D. Tourret, National Center for Scientific Research (CNRS) Solidification Summer School, St Pierre d’Oléron, France, June 2017.
20. “Design and fabrication of metallic powders for additive manufacturing at the lab scale”, M. T. Pérez-Prado, Xi’an Northwestern Polytechnical University, Xi’an, China, July 2017.
21. “Study of the deformation mechanisms of pure magnesium and magnesium alloys by EBSD-assisted slip trace analysis”, C. M. Cepeda-Jiménez, Xi’an Northwestern Polytechnical University, Xi’an, China, July 2017.
22. “Is halogen-free fire retardant low efficient?”, D.-Y. Wang, Xihua University, Chengdu, China, September 2017.
26. “In-situ mechanical characterization of materials with X-ray tomography”, F. Sket, German Aerospace Center (DLR) Department of Metals and Hybrid Materials, Cologne, Germany, October 2017.
31. “General energy-entropy-momentum integration methods for non-linear thermomechanics”, I. Romero, Department of Mechanical Engineering, Chemnitz University, Chemnitz, Germany, October 2017.

3.8. Awards

1. 2017 European Innovator (Pioneer) under 35, MIT Technology Review. Dr. R. D. Costa.
4. Elected to the Board of Directors, Society of Engineering Science (SES) Prof. J. LLorca
5. Appointed to Chairman of the European Mechanics of Materials Conference Committee (EMMCC) Prof. J. LLorca

3.9. Seminars

3. “Recent advances and challenges in Li- and post-Li- ion batteries” Prof. José Luis Tirado (from University of Cordoba). January 2017.


8. “Multi-scale mechanistic interpretations to indentation experiments across material length scales: from continuum to atomistics” Prof. Jorge Acalá (from the Polytechnic University of Cataluña). March 2017.


14. “Intramolecular singlet fission: Insights from quantum dynamical simulations” Dr. Pedro B. Coto (from Instituto de Ciencia de Materiales de Madrid (ICMM)). June 2017.

15. “High-resolution digital image correlation: Recent advances in quantifying the strain distribution at the submicron-scale” Dr. Alberto Orozco-Caballero (from University of Manchester). July 2017.


4. Training and Dissemination Activities

4.1. Theses

PhD Theses

1. “Synthesis of carbon nanomaterials by catalytic chemical vapour deposition: Growth mechanisms on metal powders and foils”
   Student: Pablo Romero
   Carlos III University of Madrid
   Advisor: Dr. Roberto Guzmán
   Date of defense: January 2017

2. “Micromechanics of Magnesium and its alloys studied by nanoindentation”
   Student: Raul Sanchez
   Carlos III University of Madrid
   Advisors: Dr. Jon Molina and Dr. Teresa Perez-Prado
   Date of defense: February 2017

3. “Standard and strain gradient crystal plasticity models: Application to Titanium”
   Student: Daniel Rodríguez
   Technical University of Madrid
   Advisor: Dr. Javier Segurado and Prof. Ignacio Romero
   Date of defense: March 2017

4. “Halogen-free Phosphorus-containing flame retardant epoxy composites”
   Student: Xiaomin Zhao
   Technical University of Madrid
   Advisors: Dr. De-Yi Wang and Prof. Javier LLorca
   Date of defense: March 2017

5. “Synthesis, structure and scalability of macroscopic carbon nanotube fibre”
   Student: Victor Javier Reguero
   Carlos III University of Madrid
   Advisor: Dr. Juan José Vilatela
   Date of defense: April 2017

6. “Prediction of mechanical properties of unidirectional FRP plies at different environmental conditions by means of computational micromechanics”
   Student: Fernando Naya
   Technical University of Madrid
   Advisor: Prof. Carlos González and Dr. Cláudio Lopes
   Date of defense: May 2017

7. “Hybrid systems based on metal oxides and nanocarbons: electronic properties and applications for photocatalysis”
   Student: Alicia Moya
   Technical University of Madrid
   Advisor: Dr. Juan José Vilatela
   Date of defense: May 2017

8. “Deformation, strengthening and fracture mechanisms of nanoscale Al/SiC multilayers”
   Student: Yang Lingwei
   Technical University of Madrid
   Advisors: Dr. Jon Molina and Prof. Javier LLorca
   Date of defense: August 2017

9. “Mechanical and multifunctional properties of polymer composites based on nano-structures”
   Student: Luis Carlos Herrera
   Carlos III University of Madrid
   Advisor: Dr. Roberto Guzmán
   Date of defense: December 2017

10. “Micromechanics of fully lamellar TiAl alloys: Effect of lamellar orientation and width”
    Student: Alberto Palomares
    Technical University of Madrid
    Advisors: Dr. Jon Molina and Dr. Teresa Pérez-Prado
    Date of defense: December 2017
Master/Bachelor Theses

1. “Evaluation of damage in composite materials by X-ray tomography: Thin plies”
   Student: Emma Largot
   National Institute of Applied Sciences of Lyon
   Advisor: Prof. Carlos González
   Date of defense: February 2017

2. “Evaluación de la capacidad de sensorización de deformación mecánica mediante fibras avanzadas”
   Student: Carlos Sánchez
   Technical University of Madrid
   Advisor: Prof. Carlos González and Dr. Cláudio Lopes
   Date of defense: March 2017

3. “Investigation on the surface treatment of textile and its flammability”
   Student: Diego Martíl
   Technical University of Madrid
   Advisor: Dr. De-Yi Wang
   Date of defense: May 2017

4. “An experimental and numerical investigation into the tensile strength of triaxially braided composites”
   Student: Alfonso García
   Technical University of Madrid
   Advisor: Dr. Alejandro García
   Date of defense: May 2017

5. “Functional fire retardant and its application in coating”
   Student: Na Li
   Technical University of Madrid & Beihang University
   Advisor: Dr. De-Yi Wang
   Date of defense: June 2017

6. “Preparations of nanocarbons and their application”
   Student: Hansong Liu
   Technical University of Madrid & Beihang University
   Advisor: Dr. De-Yi Wang
   Date of defense: June 2017

7. “Development of a continuum damage model for woven composites”
   Student: Carlos Gamir
   Delft University of Technology
   Advisor: Dr. Cláudio Lopes
   Date of Defense: June 2017

8. “Determinación del ángulo de contacto y la tensión superficial en resinas utilizadas en la fabricación de materiales compuestos”
   Student: Luis Alejandro Araujo
   Technical University of Madrid
   Advisor: Dr. Federico Sket
   Date of defense: June 2017

9. “Numerical simulation of impact on advanced configurations of composite materials”
   Student: Laura Fuentes
   Carlos III University of Madrid
   Advisor: Prof. Carlos González and Dr. Cláudio Lopes
   Date of defense: October 2017

10. “Ensayos de tracción a diferentes velocidades de deformación en laminados carbono-epoxi”
    Student: Laura Sánchez Pérez
    Technical University of Madrid
    Advisor: Prof. Carlos González
    Date of defense: July 2017

11. “Fire retardant PLA nanocomposites”
    Student: Siqi Chen
    Technical University of Madrid & Tongji University
    Advisor: Dr. De-Yi Wang
    Date of defense: July 2017
12. “Ensayos de simulación termomecánica en el Stma Gleeble 3800, ensayos mecánicos. Caracterización de microestructura de aceros”
   Student: Miguel Ángel Buendía
   Technical University of Madrid
   Advisor: Dr. Ilchat Sabirov
   Date of defense: July 2017

13. “The behavior of different materials under impact loading especially in the aeronautical industry”
   Student: Samuel Fernández
   Technical University of Madrid
   Advisor: Dr. Cláudio Lopes
   Date of defense: July 2017

14. “Simulación de un proceso de laminación acumulativa de circonio puro y comparación de su microestructura con la de un proceso de laminación convencional”
   Student: Alfonso Torijano
   Carlos III University of Madrid
   Advisor: Dr. Teresa Pérez Prado
   Date of defense: July 2017

15. “Fatigue behavior of advanced high strength steels by quenching and partitioning”
   Student: Antonio Vicente
   Technical University of Madrid
   Advisor: Dr. Ilchat Sabirov
   Date of defense: September 2017

16. “Cinética de precipitación en aleaciones de Al-Cu”
   Student: Alejandro Rodríguez
   Technical University of Madrid
   Advisor: Prof. Javier LLorca
   Date of defense: September 2017

18. “Caracterización de superaleaciones base Co para aplicaciones en ambientes extremos”
   Student: Jesús Cano
   Carlos III University of Madrid
   Advisor: Dr. Mónica Campos
   Date of defense: October 2017

4.2. Internships / Visiting Students

1. “Improvement of interfacial properties of carbon nanotube fibres”
   Student: Daniel Iglesias
   Advisor: Dr. Juan José Vilatela
   Visiting student from: Trieste University
   Period: February 2017 - March 2017

2. “Fabrication of Si-C hybrid electrodes”
   Student: David Ovejero
   Advisor: Dr. Vinod Etacheri
   Visiting student from: UAM
   Period: February 2017 - May 2017

3. “Fabrication of fire-resistant coating on paper and wood”
   Student: Ainoa Paradelo
   Advisor: Dr. De-Yi Wang
   Visiting student from: Rey Juan Carlos University
   Period: February 2017 - June 2017

4. “Effects of grain refinement”
   Student: Patricia Mazón
   Advisor: Dr. Ilchat Sabirov
   Visiting student from: Technical University of Madrid
   Period: February 2017 - June 2017

5. “Flame retardancy of natural fiber reinforced polylactic acid”
   Student: Arthur Ollivier
   Advisor: Dr. De-Yi Wang
   Visiting student from: Ecole Nationale Superior de Chemie de Lille
   Period: June 2017 - July 2017
6. “New generation fire safety polymer foams”  
Student: Louise Dupé  
Advisor: Dr. De-Yi Wang  
Visiting student from: Ecole Nationale Superior de Chemie de Lille  
Period: June 2017 - July 2017

7. “Multiscale simulation of woven composites”  
Student: Hugo Leyet  
Advisor: Prof. Carlos González and Dr. Cláudio Lopes  
Visiting student from: Rennes University  
Period: March 2017 - July 2017

8. “Crecimiento hidrotérmico del Co3O4”  
Student: Iván Jiménez  
Advisor: Dr. Vinod Etacheri  
Visiting student from: Rey Juan Carlos University  
Period: January 2017 - July 2017

9. “Demostrador de un circuito sensor para detector el flujo de resina en la fabricación de materiales compuestos”  
Student: Raúl Sanz  
Advisor: Prof. Carlos González  
Visiting student from: Technical University of Madrid  
Period: June 2017 - July 2017

10. “Fabricación de materiales compuestos”  
Student: Alba Clemente  
Advisor: Prof. Carlos González  
Visiting student from: Technical University of Madrid  
Period: June 2017 - July 2017

11. “Caracterización de recubrimientos a diferentes temperaturas”  
Student: Antonio Villahermosa  
Advisor: Dr. Jon Molina  
Visiting student from: Complutense University of Madrid  
Period: February 2017 - August 2017

12. “Multifunctional nanocomposites”  
Student: Rodrigo Cárdenas  
Advisor: Dr. Juan José Vilatela  
Visiting student from: Iberoamericana University  
Period: June 2017 - August 2017

13. “Tareas dentro de la línea de fabricación aditiva de materiales metálicos. Estudio del potencial de varias aleaciones de aluminio para ser procesadas por impresión 3D”  
Student: Carlota Ferrer  
Rey Juan Carlos University  
Advisor: Dr. Teresa Pérez Prado  
Date of defense: March 2017 - August 2017

14. “Preparation of properties of high performance polymer composites”  
Student: Alejandro Jimenez  
Advisor: Dr. De-Yi Wang  
Visiting student from: University of Sevilla  
Period: June 2017 - August 2017

15. “Study liquid and polymer interaction with macroscopic ensembles of nanobuilding blocks”  
Student: Rahul Ramakrishnan  
Advisor: Dr. Juan José Vilatela  
Visiting student from: MIT  
Period: June 2017 - August 2017

16. “Metallic alloys in in structural applications that involve high stresses and temperatures”  
Student: Jun Lian Wang  
Advisor: Dr. Javier Segurado  
Visiting student from: Technical University of Madrid  
Period: June 2017 - August 2017

17. “Monotonous and cycling behaviour of refractory materials used in furnaces for iron- and steel-making”  
Student: Santiago Rodriguez  
Advisor: Dr. Ilchat Sabirov  
Visiting student from: Technical University of Madrid  
Period: June 2017 - August 2017
18. “Design testing and simulation of advanced composites”
   Student: Héctor Navarro
   Advisor: Dr. Cláudio Lopes
   Visiting student from: Universidad de Valencia
   Period: June 2017 - September 2017

   Student: Dieter Plessers
   Advisor: Dr. Ruben Costa
   Visiting student from: KU Leuven
   Period: June 2017 - September 2017

20. “Construcción de Relaciones estructura-propiedad a través de técnicas informáticas”
   Student: Juan Manuel Moreno
   Advisor: Dr. Maciej Haranczyk
   Visiting student from: Complutense University of Madrid
   Period: August 2017 - November 2017

   Student: Karla Garrido
   Advisor: Dr. Juan Pedro Fernández
   Visiting student from: Universidad de Concepción
   Period: September 2017 - December 2017

22. “High resolution microstructural and structural analysis of Ti_{6}Al_{4}V specimens”
   Student: Francesco Potenza
   Advisor: Dr. Teresa Pérez Prado
   Visiting student from: Trento University
   Period: September 2017 - December 2017

23. “Simulation of the mechanical behavior of magnesium alloys using polycrystalline homogenization techniques”
   Student: Mohammad Jalili
   Advisor: Dr. Javier Segurado
   Visiting student from: Kashan University
   Period: October 2017 - December 2017

24. “Fire properties of PLA nanocomposites”
   Student: Pengcheng Zao
   Technical University of Madrid & Tongji University
   Advisor: Dr. De-Yi Wang
   Date of defense: November 2017 - December 2017

4.3 Teaching in Masters

1. “Simulation in materials engineering”
   Master in Materials Engineering, Technical University of Madrid
   Professor: Dr. Cláudio Lopes

2. “Polymer for advanced applications”
   Master in Materials Engineering, Technical University of Madrid
   Professor: Dr. De-Yi Wang

3. “Nanocomposites”
   Master in Materials Engineering, Technical University of Madrid
   Professor: Dr. De-Yi Wang

4. “Structural characterization of materials I/”
   Master in Materials Engineering, Technical University of Madrid
   Professor: Dr. Federico Sket

5. Metal matrix composites”
   Master in Composite Materials, Technical University of Madrid - AIRBUS
   Professor: Dr. Ilchat Sabirov

6. “Hierarchical composites”
   Master in Composite Materials, Technical University of Madrid - AIRBUS
   Professor: Dr. Juan José Vilatela

7. “Advanced composite materials”
   Master in Materials Engineering, Carlos III University of Madrid
   Professor: Dr. Jon Mikel Molina
8. “Simulation techniques of materials”
   Master in Materials Engineering, Carlos III University of Madrid
   Professor: Dr. Jon Mikel Molina

9. “Materials science and engineering”
   Master in Materials Engineering, Carlos III University of Madrid
   Professor: Dr. Juan José Vilatela

10. “Technology applied to nanomaterials”
    Master in Muchanic Engineering, Carlos III University of Madrid
    Professor: Dr. Juan José Vilatela

11. “Aerospace materials I”
    Master in Materials Engineering, Carlos III University of Madrid
    Professor: Dr. Srdjan Milenkovic

12. “Aerospace materials II”
    Master in Materials Engineering, Carlos III University of Madrid
    Professor: Dr. Srdjan Milenkovic

13. “Thermal and thermomechanical testing of materials”
    Master in Materials Engineering, Carlos III University of Madrid
    Professor: Dr. Srdjan Milenkovic

4.4. Institutional Activities

1. Member of the European Materials Modelling Council (EMMC)

2. Member of the European Materials Characterization Council (EMCC)

3. Member of the European Energy Research Alliance (EERA AISBL)

4. Member of the Executive Committee of the Spanish Association for Numerical Methods in Engineering (SEMNIA)

5. Council Member of the International Association for Computational Mechanics (IACM)

6. Member of the Strategic Expert Group of the M-Eranet, H2020 - European Commission

7. Member of the European Composites, Plastics and Polymer Processing Platform (ECP4)

8. Local Contact Point of the EURAXESS pan-European initiative

9. Technical Secretariat of the Spanish Technological Platform of Advanced Materials and Nanomaterials (MATERPLAT)

10. Member of the Board of Directors of the Spanish Association of Composite Materials (AEMAC)

11. Member of the Board of Directors of the Spanish Materials Society (SOCIEMAT)

12. Member of the Spanish Aerospace Platform

13. Member of the Spanish Technological Platform for Advanced Manufacturing

14. Member of the Technological Clusters on Aerospace, Security and Renewable Energies promoted by Madrid Network.

15. Member of the Network of Research Laboratories of Comunidad de Madrid (REDLAB)
4.5. Outreach

1. Participation in the “International Day of Women and Girls in Science”, promoted by Fundación Madri+d.

2. Participation in the “Science Week Madrid 2017”, promoted by Fundación Madri+d.


4. Participation in the “Graphene Market Place”, promoted and organised by AIRBUS

5. Collaboration with Formula Student UC3M team

6. Organisation of primary-secondary school and bachelor-master students visits to IMDEA Materials Institute