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...

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IMDEA Materials Institute

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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:**

science

excellence in materials science and engineering research

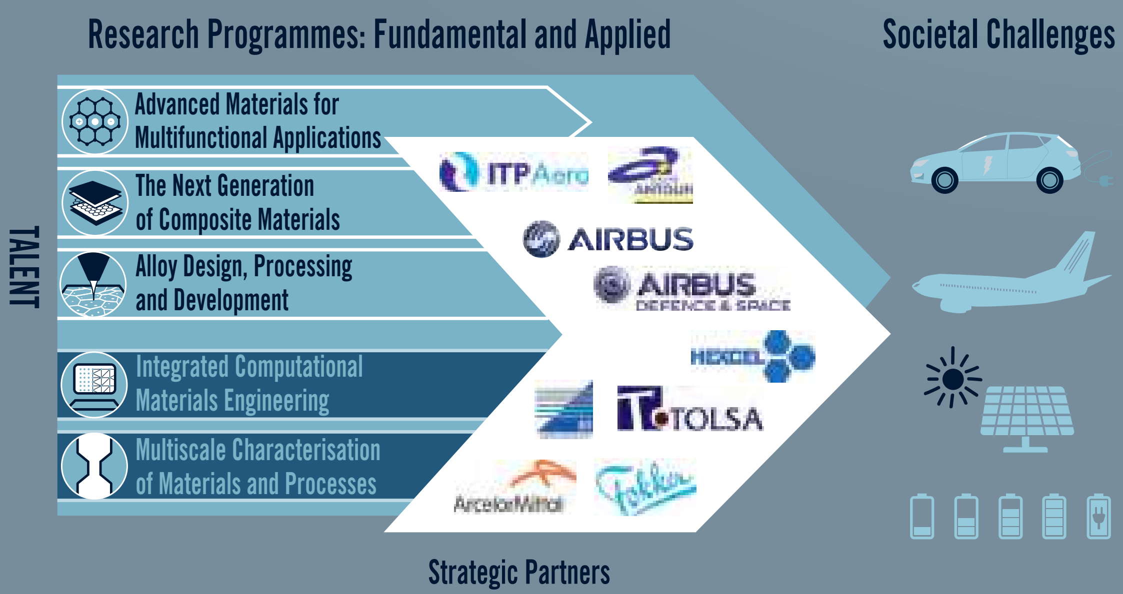
transfer

technology **transfer** to industry to increase competitiveness and maintain technological leadership

talent

attraction of talented researchers from all over the world to Madrid to work in an international and interdisciplinary environment

The IMDEA Materials Institute has an **stablished 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.



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.

116 researchers

16 nationalities

50% PhDs

40% foreign researchers

16 research groups

The facilities of IMDEA Materials Institute

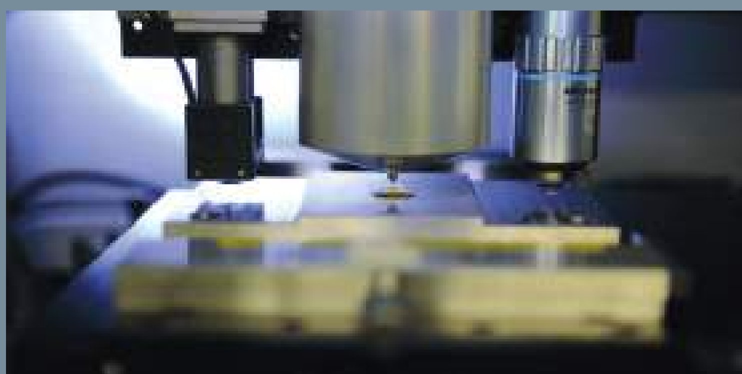
The building and laboratories of IMDEA Materials Institute are located at the Scientific and Technological Park of the Technical University of Madrid in Tecnogetafe, Madrid.

2.640 m^2 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.**



our structure

EXECUTIVE BOARD

- DIRECTOR
- DEPUTY DIRECTOR

RESEARCH PROGRAMMES

- ADVANCED MATERIALS FOR MULTIFUNCTIONAL APPLICATIONS
- THE NEXT GENERATION OF COMPOSITE MATERIALS
- NOVEL ALLOY DESIGN, PROCESSING AND DEVELOPMENT
- INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING
- MULTISCALE CHARACTERISATION OF MATERIALS AND PROCESSES

GENERAL MANAGEMENT

- Human Resources
- Financial Management
- Proposals
- Project Management
- Technology Transfer
- IT Management
- Events
- Infrastructure and Facilities Management

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in figures

human resources

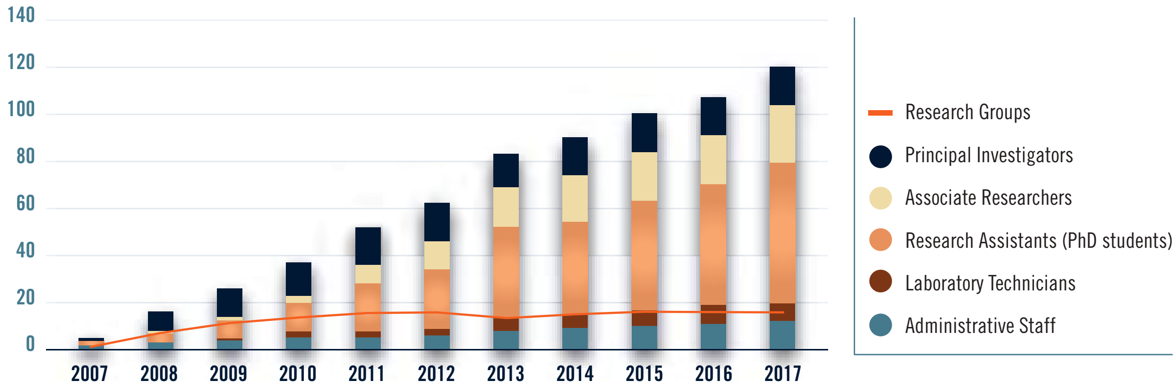
talent

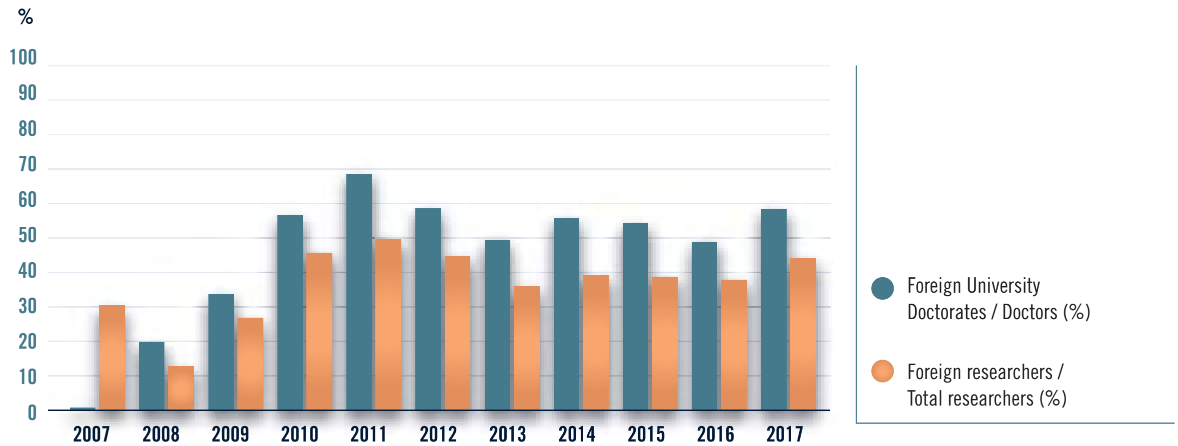
Talent attraction has been the key to the Institute´s **success**.

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**

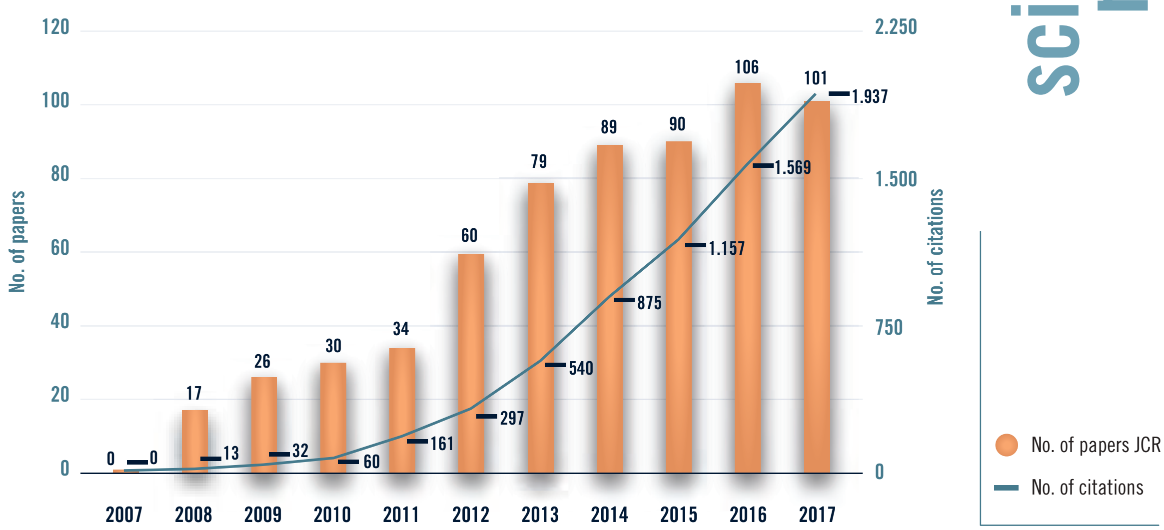
24 defended PhD theses since 2007

64 ongoing PhD theses

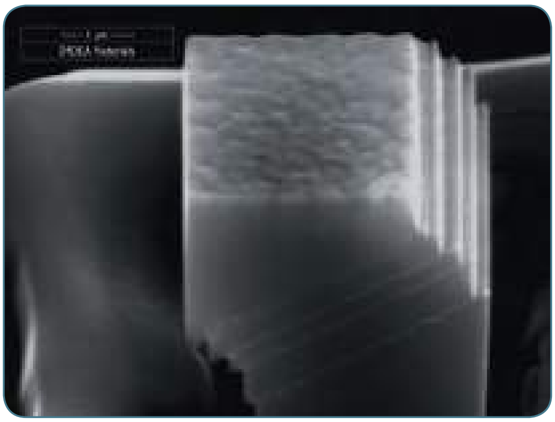
scientific results

science

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



in figures

29 keynote/ invited talks

101 JCR papers

40 invited seminars

5 patents applied

1937 number of citations

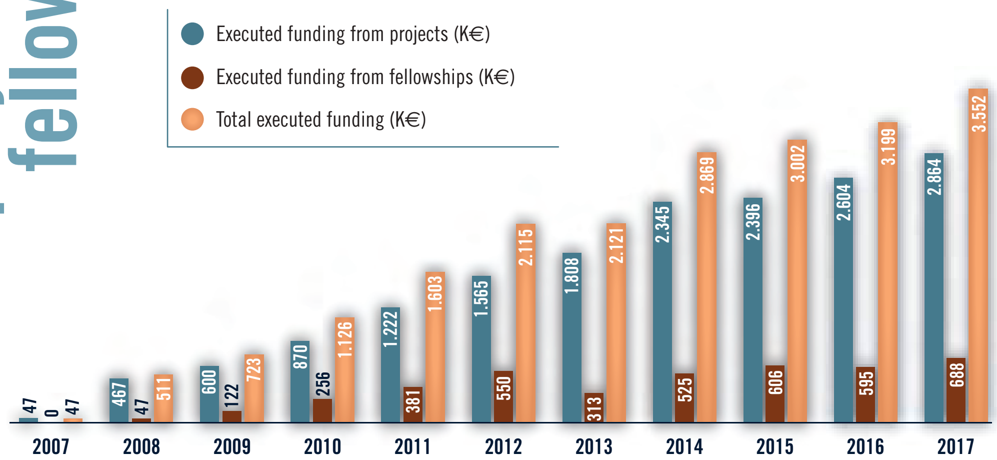
transfer

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.

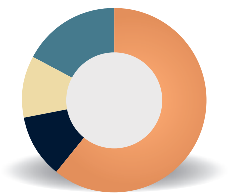
Companies which had active collaboration with IMDEA Materials during 2017

projects and fellowships

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%

in figures

44
R&D projects

2
ERC projects running

17
R&D contracts with companies

10 years of success

2007

Launch of IMDEA Materials Institute

2008



Temporary facilities at the Technical University of Madrid

First European Project. MAAXIMUS

2009

Temporary facilities at the Carlos III University of Madrid

First industrial R&D contracts


2010


The begining of the final site construction

2012

Final site inauguration

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**

2013

carinhyph
Bottom-up fabrication of nano carbon-inorganic hybrid materials for photocatalytic hydrogen production

SEVENTH FRAMEWORK PROGRAMME

First European Project coordinated by IMDEA Materials Institute. CARINHYPH

Launch of Research Programmes

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

2015

First European Research Council (ERC) Project. VIRMETAL

European Commission

HORIZON 2020

erc
European Research Council

2016

MARIE CURIE ACTIONS

First International Training Network within Marie Curie Programme - DYNACOMP

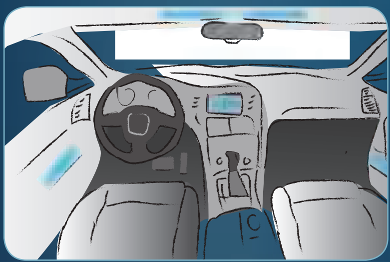
2017

research

talent science transfer

research

Advanced Materials for Multifunctional Applications

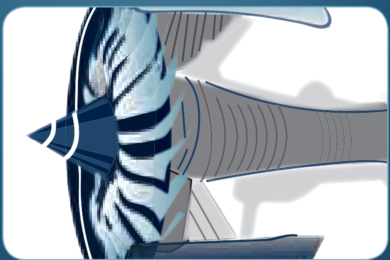


- Synthesis and integration of nanomaterials and polymer-based multifunctional nanocomposites
- New materials and strategies for electrochemical energy storage and conversion
- Hybrid optoelectronic materials and sustainable lighting devices
- Computational and data-driven materials discovery

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. Sensoring and Industry 4.0
- Multifunctional capabilities (fire resistance, electrical, thermal, sensing, energy management, health monitoring...)

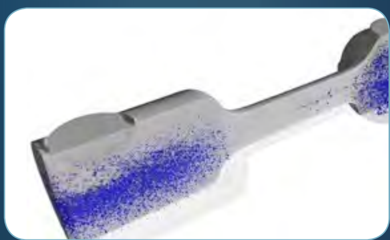
Novel Alloy Design, Processing and Development



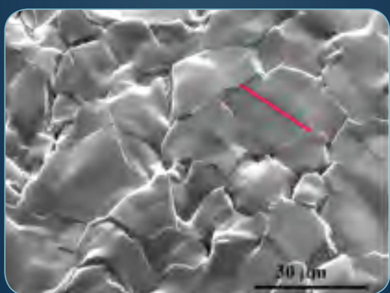
- Structural alloys: light alloys, high temperature alloys and high strength steels
- Characterisation of microstructure and mechanical behaviour
- Advanced Manufacturing: solidification and casting, physical simulation of metallurgical processes (rolling, forging, extrusion...)
- Additive manufacturing: 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…)

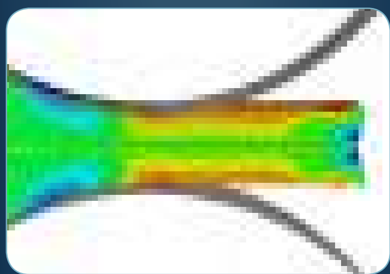


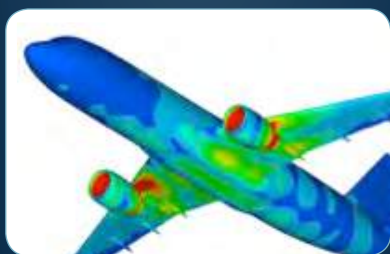
- **4D characterisation:** In-situ characterisation of deformation and processes across multiple length scales (750ºC)



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

talent science transfer

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 thermosplastics.
- 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.

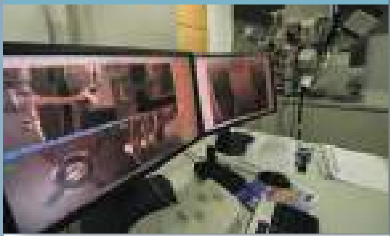
Energy storage and conversion devices

- 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-O_2, Na-ion, and hybrid batteries etc.).
- Fabrication and testing of nanocarbon-based electrodes and their integration with liquid and solid electrolytes to form large-age (> 100 cm^2) 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

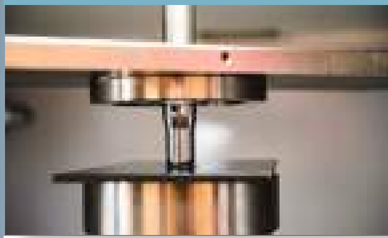
- Fabrication and characterisation of hybrid light-emitting diodes and thin-film lighting devices.
- Rack system consisting of 7 positions that are independently driven, while the luminance and chromaticity features are monitored over time via UV-VIS spectrophotometers coupled to integrated spheres.
- 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



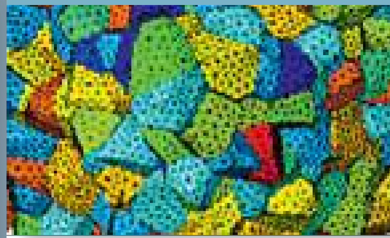
- 3D microscopy at different length-scales, including X-ray tomography, 3D-SEM, 3D-EDS and 3D-EBSD in the FIB and 3D-TEM and 3D-EDS in the TEM.
- In-situ mechanical testing of mininaturised samples in the X-ray tomography system as well as in the SEM and TEM.
- In-situ processing studies in the X-ray tomography system, such as casting, infiltration and curing of polymer based materials.
- Raman spectrophotometer.

Mechanical properties



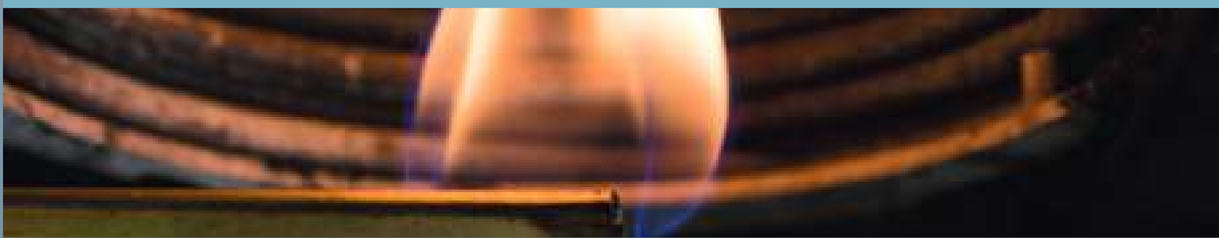
- Mechanical testing of a wide range of materials, using electromechanical and hydraulic machines (quasi-static, dynamic, fracture and fatigue testing in a wide range of temperatures).
- Characterisation of mechanical properties at multiple length scales, including nanoindentation, micropillar compression, microtensile testing and fracture micromechanics.
- Tests can be carried out both ex-situ and in-situ in SEM, TEM and X-ray tomography including measurements at elevated temperature.

Simulation



- Simulation techniques at different scales (electronic, atomistic, mesoscopic and continuum) to design or improve materials and components by means of virtual testing and virtual processing.
- High-performance computer cluster (600+ Intel Xeon CPU cores and NVIDIA GPU acceleration leading to a computational power of 90 Tflops).
- In-house developed simulation tools.
- Commercial and open source software tools for modelling and simulation in Materials Science and Enginnering (CALPHAD, DICTRA, Micress, Abaqus, LS-Dyna, PamCrash, LAMMPS, etc.).

Functional properties



Fire resistance

- Rapid laboratory scale tests for screening (micro-scale combustion calorimetry and oxygen index).
- Dual cone calorimetry and UL94 Horizonal/Vertical Flame Chamber.

Thermal

- DSC, TGA and Hot Disk Thermal Conductivity analyse. Thermal behaviour of mechanical properties, DMA and rheology. Horizontal
- Pushrod Dilatomer for the measurement of dimensional changes.

Electrochemical

- Electrochemical characterisation of energy storage devices (Li-ion, Li-S, Li-O$_2$, Na-ion, and hybrid batteries). Simultaneous testing of 100 batteries can be performed using multichannel battery testers.
- 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.
- Time-Correlated Single Photon Counting using a laser excitation module.

programme

Advanced Materials for Multifunctional Applications

Goal and vision

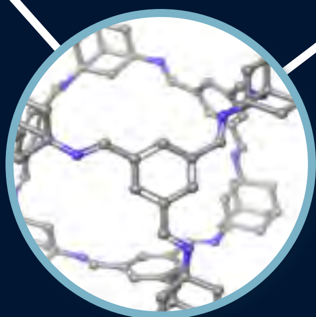
The Programme on Advanced Materials for Multifunctional Applications at IMDEA Materials Institute combines expertise in design and synthesis of nano and molecular building blocks with their integration into macroscopic materials and devices. The guiding objective is to simultaneously realise various 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 (MoS_2), nanocarbon, nano metal hydroxide, nanocoatings, 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

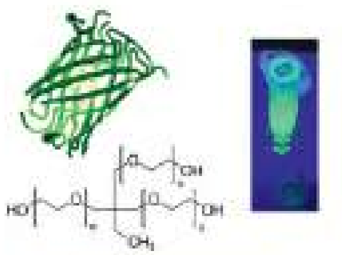
- Tailored designing of nanostructured electrode materials, interfaces and electrolyte compositions.
- Spectroscopic/microscopic studies and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O_2.

Computational and data-driven materials discovery

- Discovery of porous materials for energy applications (CO_2 capture, methane storage).
- Design of ionic liquids.
- Characterisation of nanoparticles and others.

Concept of CNT fibre as current collectors/active material for energy management devices

Active material for electrodes



Stabilisation of luminescent proteins in polymers for optoelectronic applications

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.

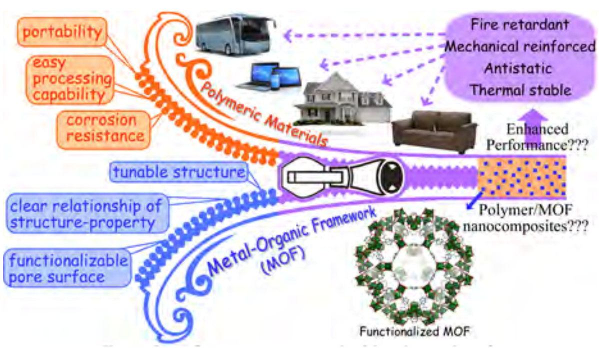


Figure 1. Illustration of composite materials with enhanced performance.

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.

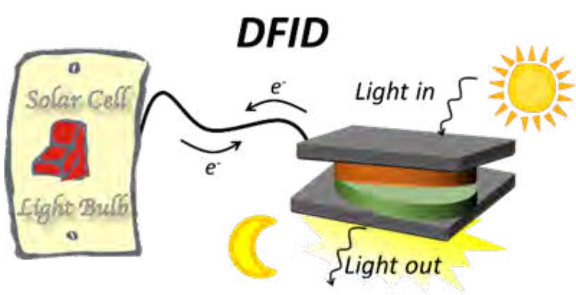


Figure 2. Schematic concept of DFID project.

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.

Reference: Bianka M. D. Puscher, Meltem F. Aygüler, Pablo Docampo, Rubén D. Costa, Advance Energy Materials 7, 2017

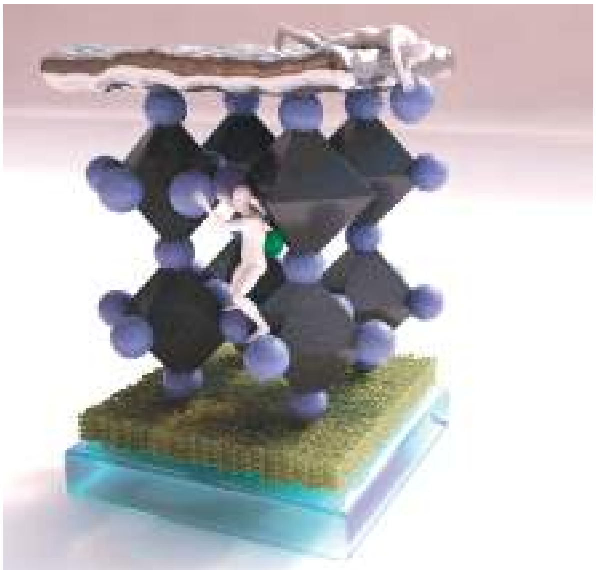


Figure 3. Schematic representation of the ionic-assisted dynamic behavior in perovskite-based devices.

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.

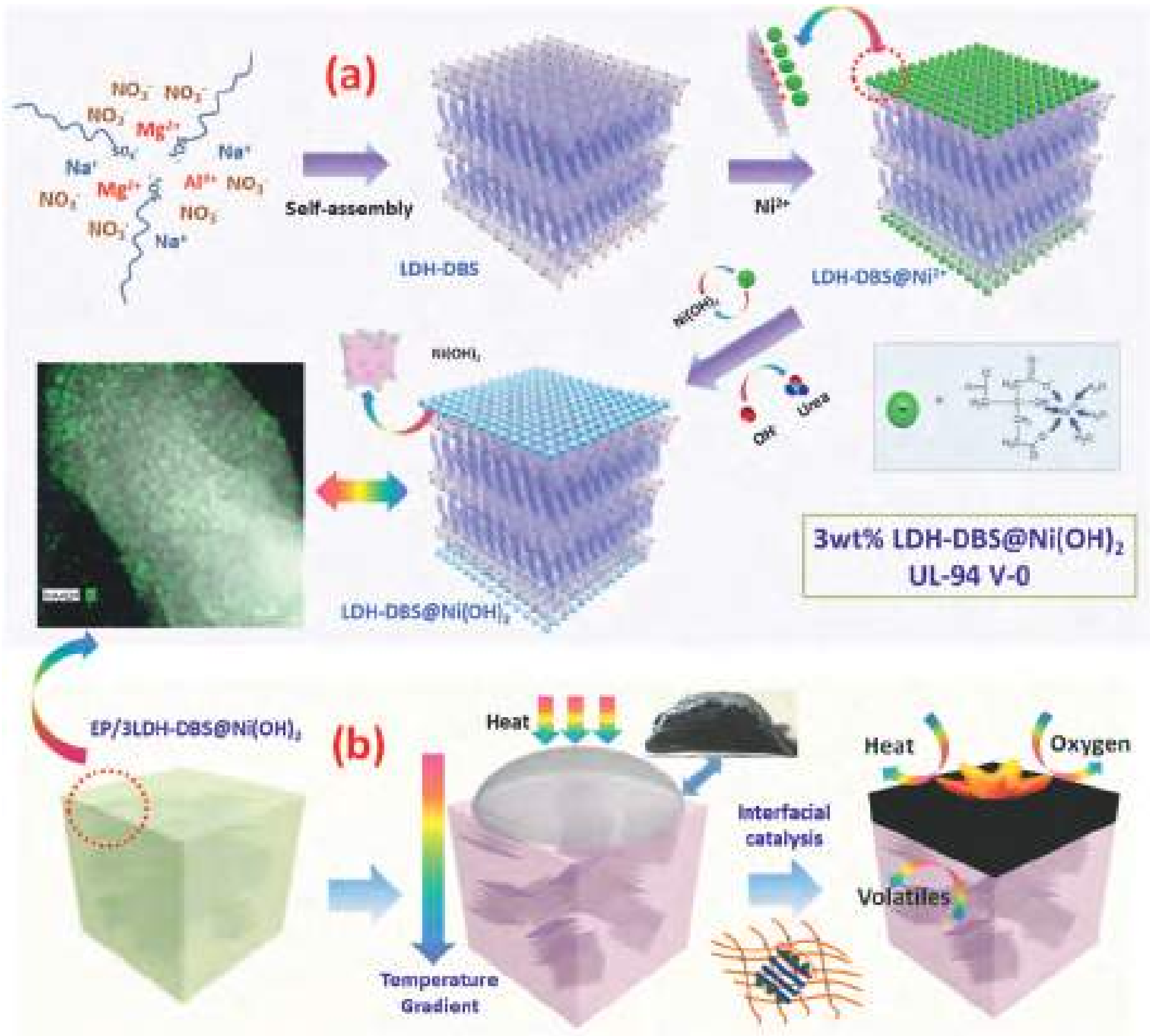


Figure 4. Scheme 1 (a) Design and synthesis of LDH-DBS@Ni(OH)$_2$; (b) interfacial charring mechanism.

References:

[1] Ye-Tang Pan, Lu Zhang , Xiaomin Zhao De-Yi Wang. Chemical Science, 8, 3399-3409, 2017.
[2] Ye-Tang Pan, Cédric Trempont, De-Yi Wang. Chemical Engineering Journal, 330, 1222-1231, 2017.
[3] Zhi Li, Lejing Liu, Alejandro Jiménez González, De-Yi Wang. Polymer Chemistry, 8, 3926-3936, 2017.
[4] Zhi Li, De-Yi Wang. Materials & Design, 2017,129, 69-81.
[5] Junhao Zhang, Qinghong Kong, De-Yi Wang. Journal of Materials Chemistry A, 2018.

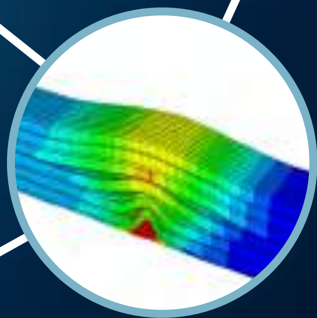
programme

The Next Generation of Composite Materials

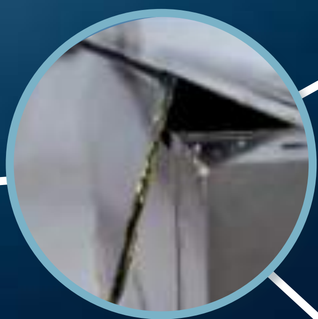
The Next Generation of Composite Materials Programme aims at developing solutions for high performance structural composites with enhanced multifunctional capabilities such as thermal, electrical and fire resistance. The programme is focused on key aspects of material science and engineering including 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.

Multifunctional Nanocomposites

High Performance Polymer Nanocomposites

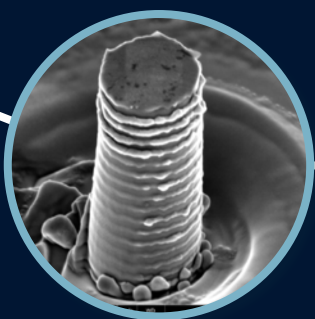


Design & Simulation of Composite Structures



Structural Composites

X-Ray Characterisation of Materials



Nanomechanics

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

- Green (recyclable) epoxies. Electric current-assisted curing for bondings and repairs. Effect of ageing on composite performance. Recycling and reuse of carbon fibre.

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

- Fire resistance. Electrical and thermal conductivity. Energy management. Barrier properties. Non-destructive evaluation and health monitoring. Sensors and smart materials.

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

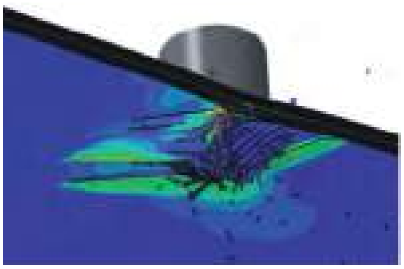
- Multiscale strategies for design and optimisation of composite materials and structures. Behaviour of composite materials and structures under high velocity impact (ice, metallic fragment or blade). Crash-worthiness and failure of composite structures. Effects of defects.

Virtual processing of composites

- Manufacturing process simulation. Multiphysics models for manufacturing including forming, injection/infusion process as well as curing. Characterisation of processing parameters.
- Simulation based smart manufacturing processes. Sensoring and process control.

Manufacturing of structural composites.

Multifunctional composites (e.g. lightning impact).



Multiscale virtual testing and processing.

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.

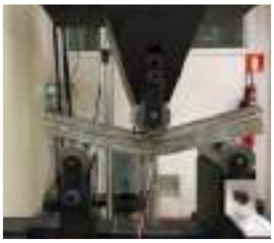


Figure 1. Fiber metal laminate (steel and glass) manufactured by UPM subjected to three-point bending (courtesy of Prof. Suárez Bermejo).

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

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 it 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 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.

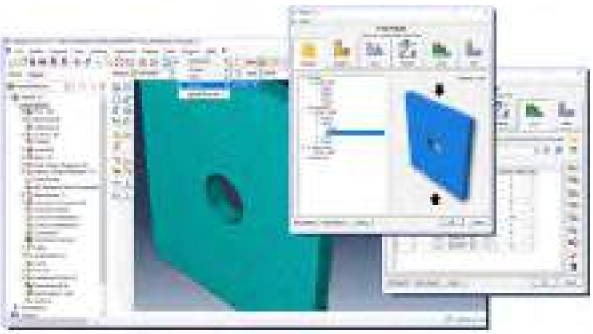


Figure 5. Graphical User Interface (GUI) of the Virtual Test Lab plug-in in the Abaqus/ CAE environment.

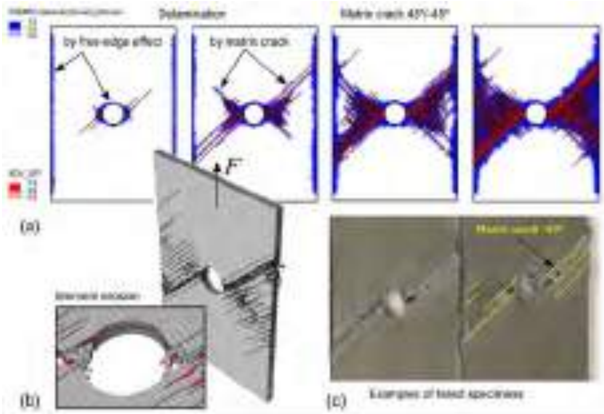


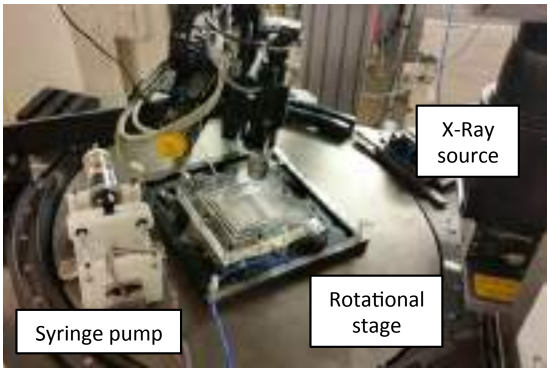
Figure 6. Experimentally-observed (c) and simulated (a; b) progression of failure mechanisms in OHT specimens of 'soft' laminates (10/80/10): (a) undeformed damage evolution of delamination and matrix cracking. b) realistic transverse cracks simulated by means of crack-band erosion. c) experimentally-observed failure modes in failed specimens (photo: Fokker).

Reference: O. Falcó et al., Composite Structures 190, 2018.

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.

(a)



(b)

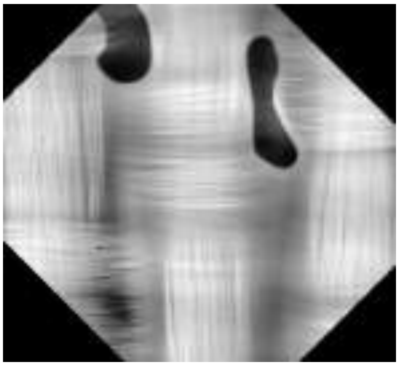


Figure 7. a) Experimental set-up for XCT imaging during resin injection of composite materials, b) XCT tomogram showing voids entrapped in a plain woven composite.

Figure 8. Fluid dynamics simulation of the flow propagation process at the micro level including viscous and capillary forces.

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).

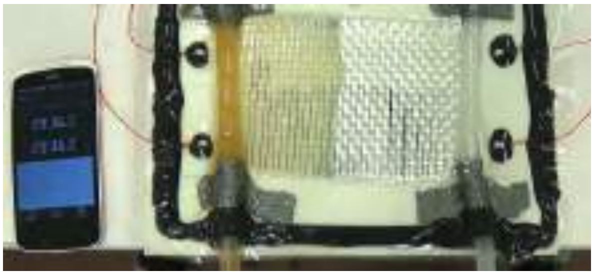
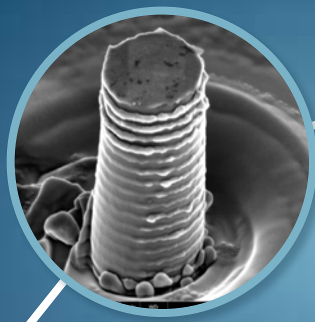


Figure 9. Infusion test with embedded CNT fibers for flow front assessment.

Figure 10. Four point bending tests of a composite material laminate with embedded CNT fiber for strain analysis.

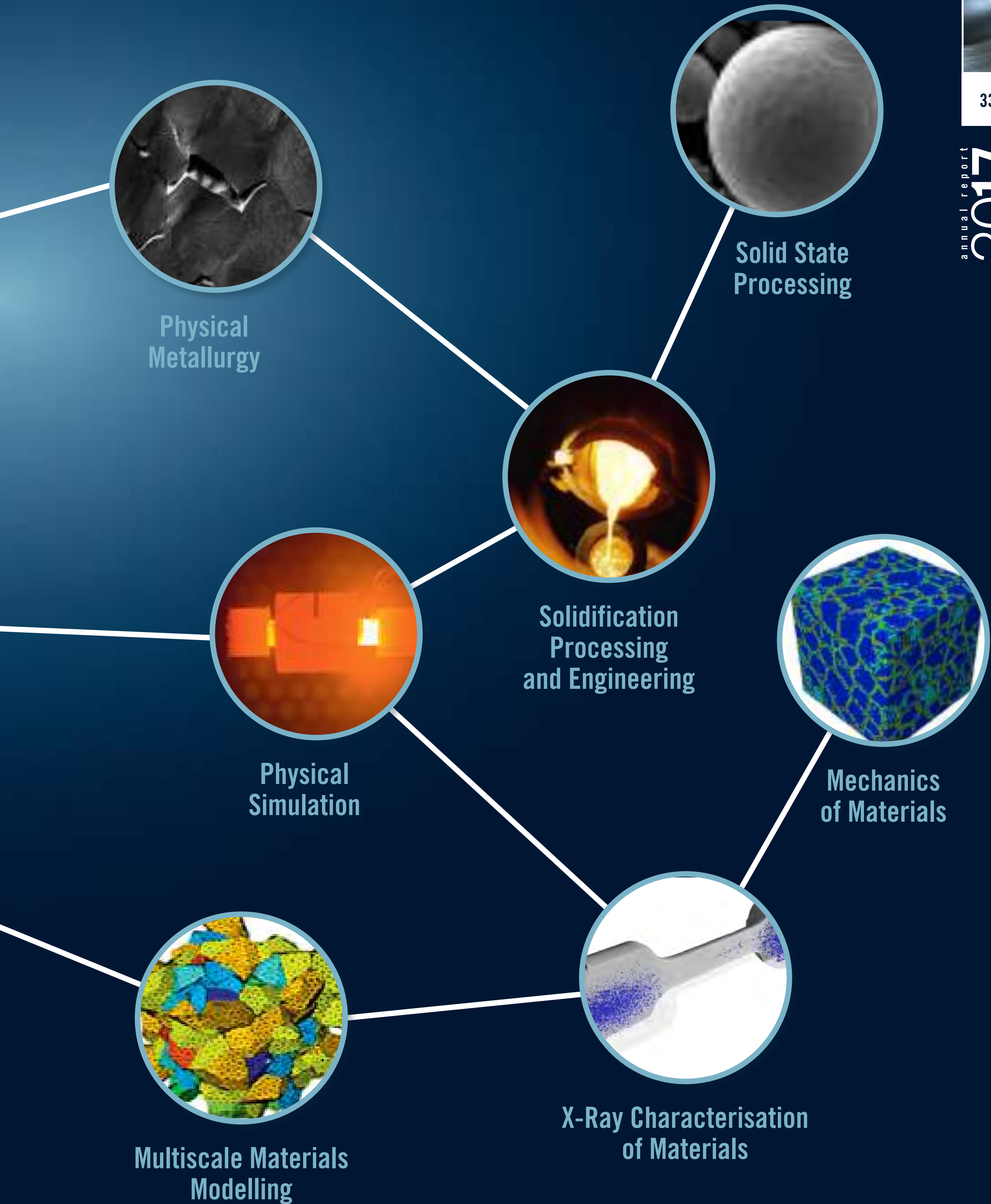
programme

Novel Alloy Design, Processing and Development



Goal and vision

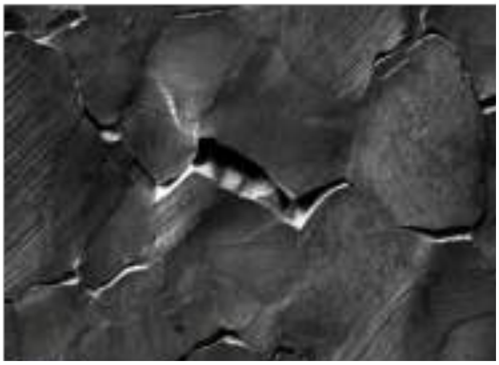
The programme, integrated by experts in physical simulation, solidification and casting, physical metallurgy, solid state processing and computational materials engineering, aims to explore the processing-structure-property relationships in metallic alloys, with special emphasis on the role of microstructure 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.


Solid State
Processing
Physical
Metallurgy
Solidification
Processing
and Engineering
Physical
Simulation
Mechanics
of Materials
X-Ray Characterisation
of Materials
Multiscale Materials
Modelling

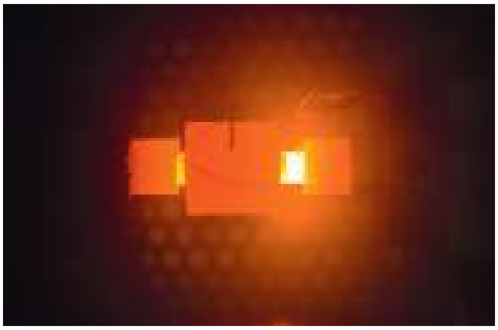
Main research lines

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.



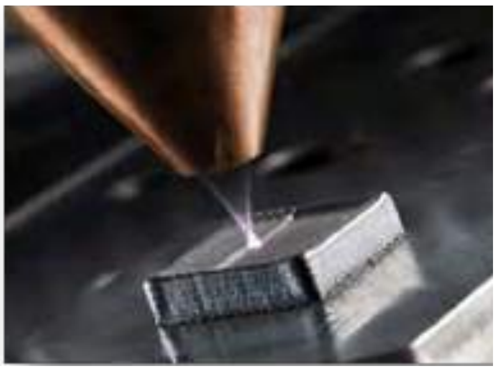
In-situ characterisation.



Advanced manufacturing.

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.



Additive manufacturing (www.industr.com).

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.

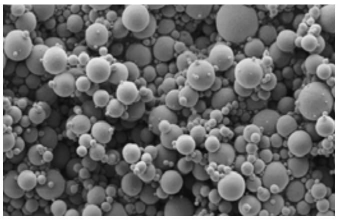


Figure 1. Aluminium powder produced by gas atomization.

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

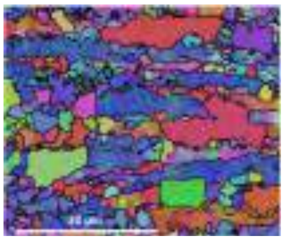
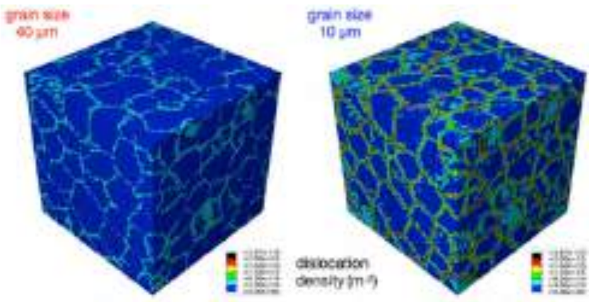


Figure 3. EBSD map of a steel after heat treatment.

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.



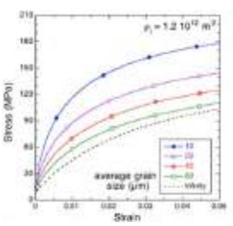


Figure 4. Stress-strain curves predicted for different grain sizes and dislocation distribution in the microstructure.

Reference: S. Haouala, J. Segurado, J. LLorca, Acta Materialia 148, 2018.

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.

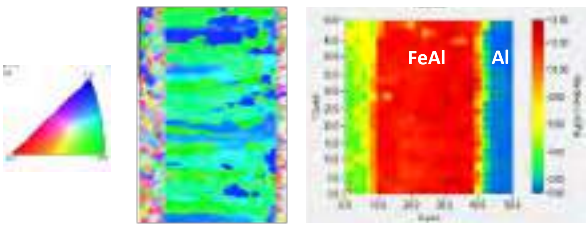
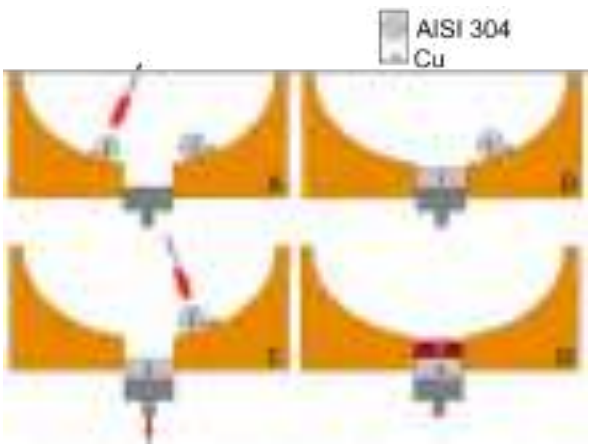
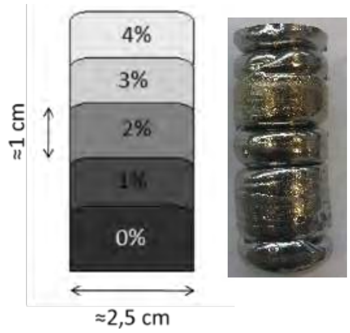


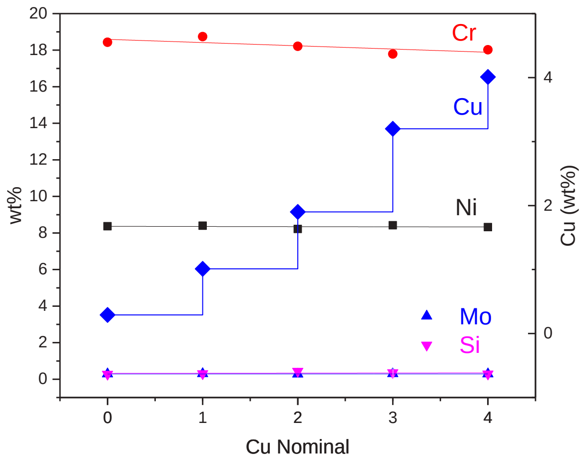
Figure 5. EBSD map of a steel/AA6061 joint (left) and nanohardness map for the present joint (right).

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.







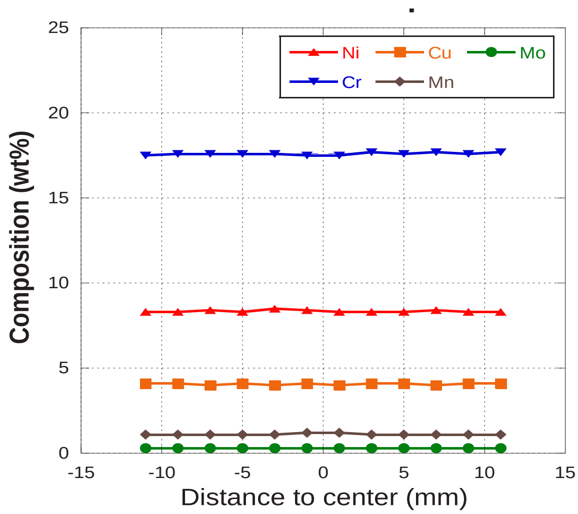


Figure 6. Schematic of the method, ingots produced with their overall composition and homogeneity along the sample.

Reference: M.Cristobal, D. San-Martin, C. Capdevila, J. A. Jimenez, S. Milenkovic, Journal of Materials Research and Technology, in press.

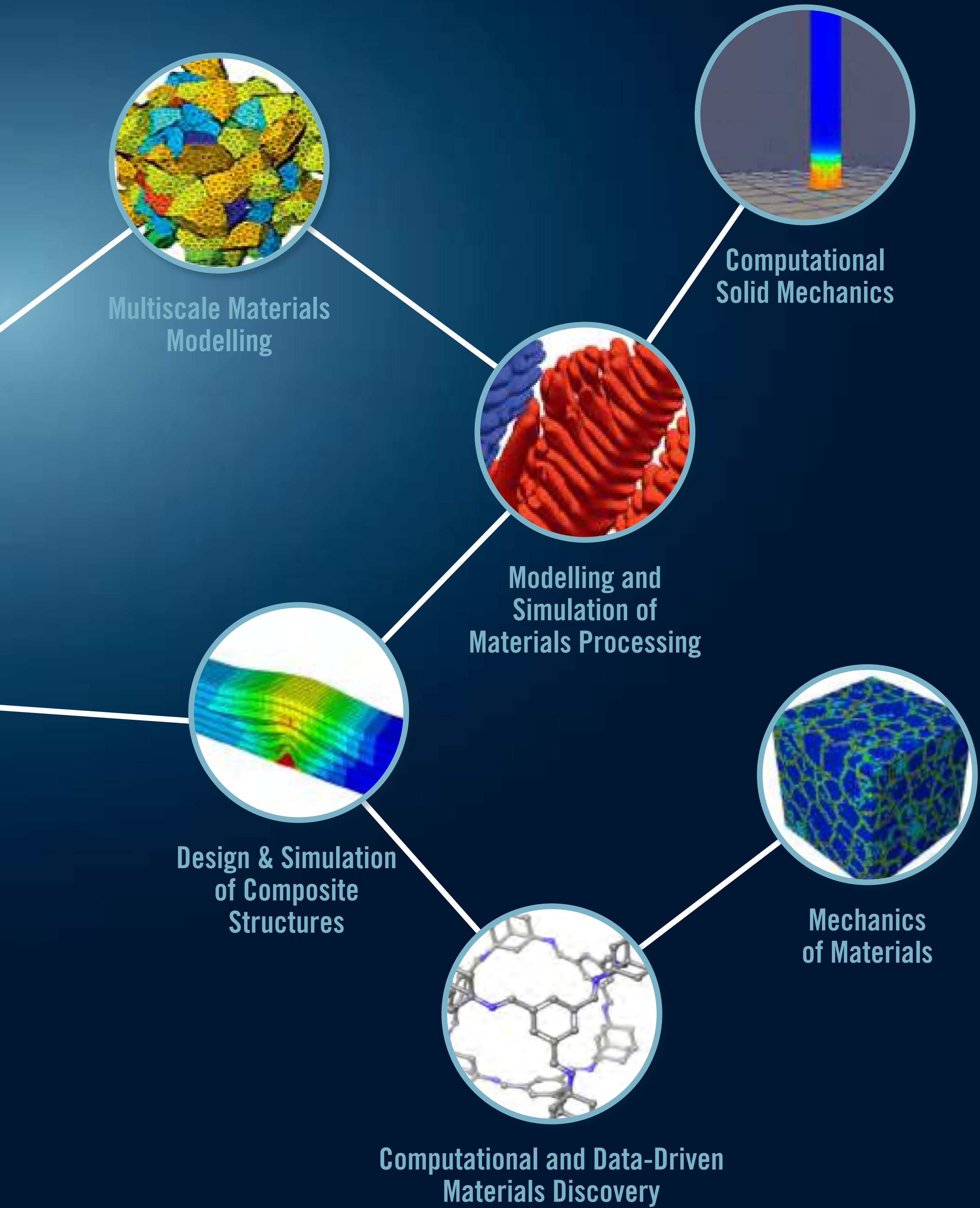
programme

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, mesocopic 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

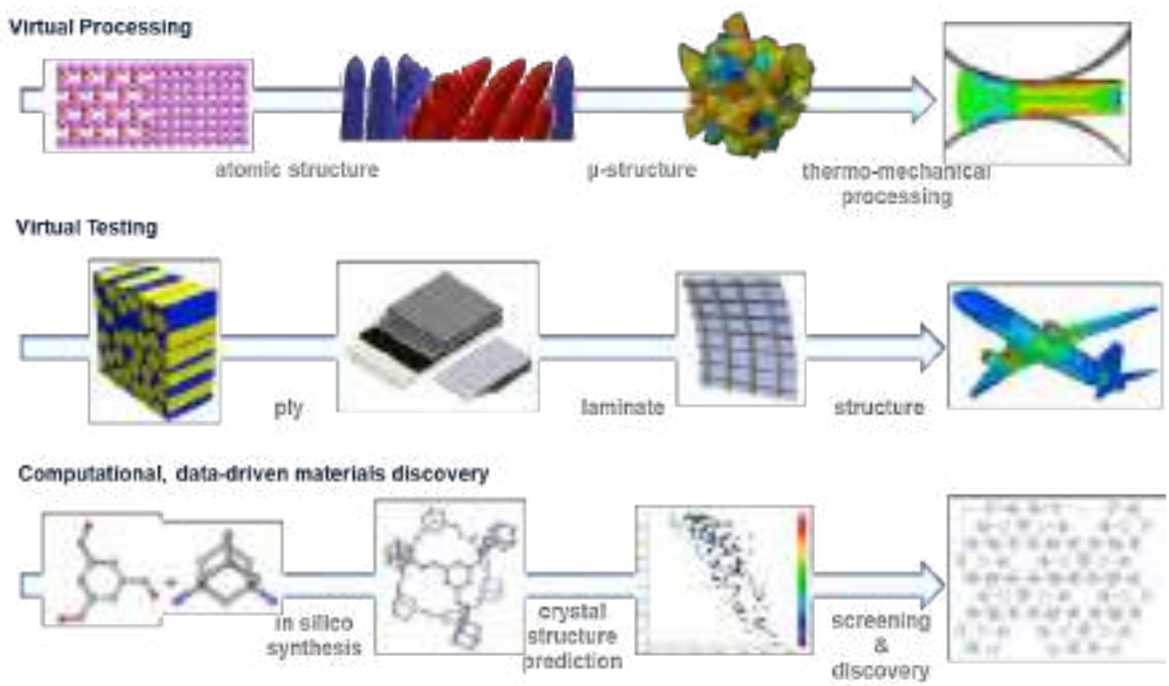
- Light (Al, Mg and Ti) metallic alloys and their composites. Ni-based superalloys. Multifunctional composite materials and structures. Materials for energy generation and storage.

Materials modelling at different length and time scales

- First principles calculations. Molecular mechanics and molecular dynamics. Dislocation dynamics. Object and lattice Kinetic Monte Carlo. Computational thermodynamics and kinetics. Phase field. Multiscale modelling of dendritic growth (dendritic needle network approach). Numerical methods for solids (finite elements and other approximations for solid mechanics). Computational micromechanics. Computational mechanics. Material informatics for analysis of large material datasets. Data-driven materials design.

Multiscale materials modelling

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



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,

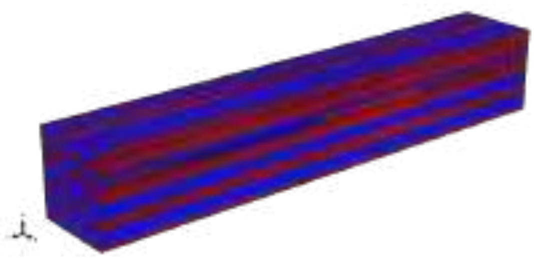


Figure 1. 3D Representative Volume Element (RVE) to study the process of fracture in hybrid composites.

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.

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 θ' (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 θ' 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 θ' 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 θ' 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.

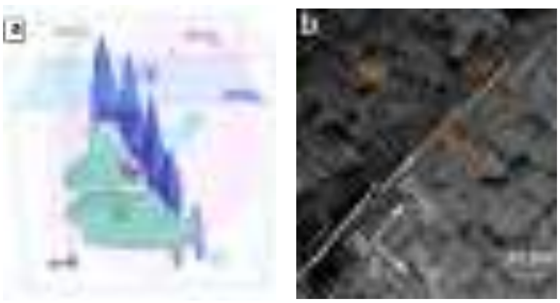


Figure 2. (a) Multiscale simulation of the nucleation and growth of θ' (Al2Cu) precipitates on dislocations during high temperature aging of an Al-Cu alloy. (b) Transmission electron microscopy micrograph showing the formation of a staircase structure of θ' precipitates on a dislocation. From H. Liu,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

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.

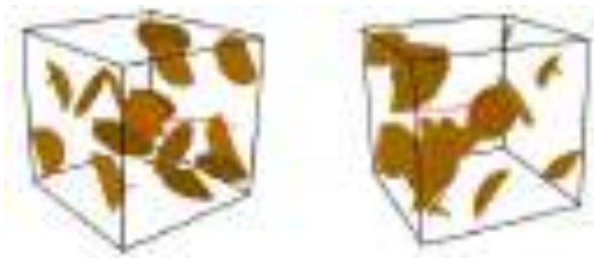


Figure 3. Dislocation dynamics simulation of the propagation of a dislocation through a forest of θ' precipitates in an Al-Cu alloy.

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.

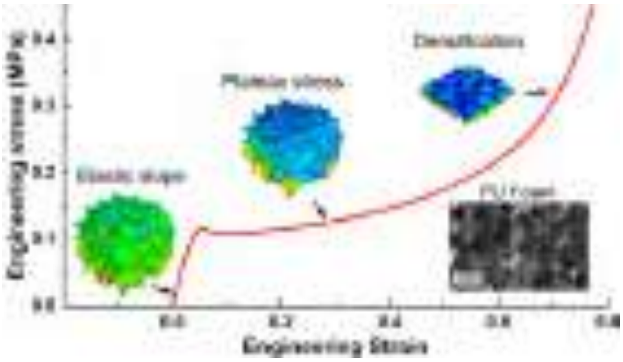


Figure 4. Progressive simulation of the compressive behaviour of PU foams. The RVE approach is used to predict different stages of applied strain: elastic behaviour, plateau stress and foam densification.

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*)

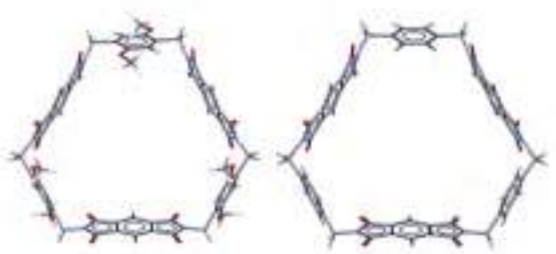


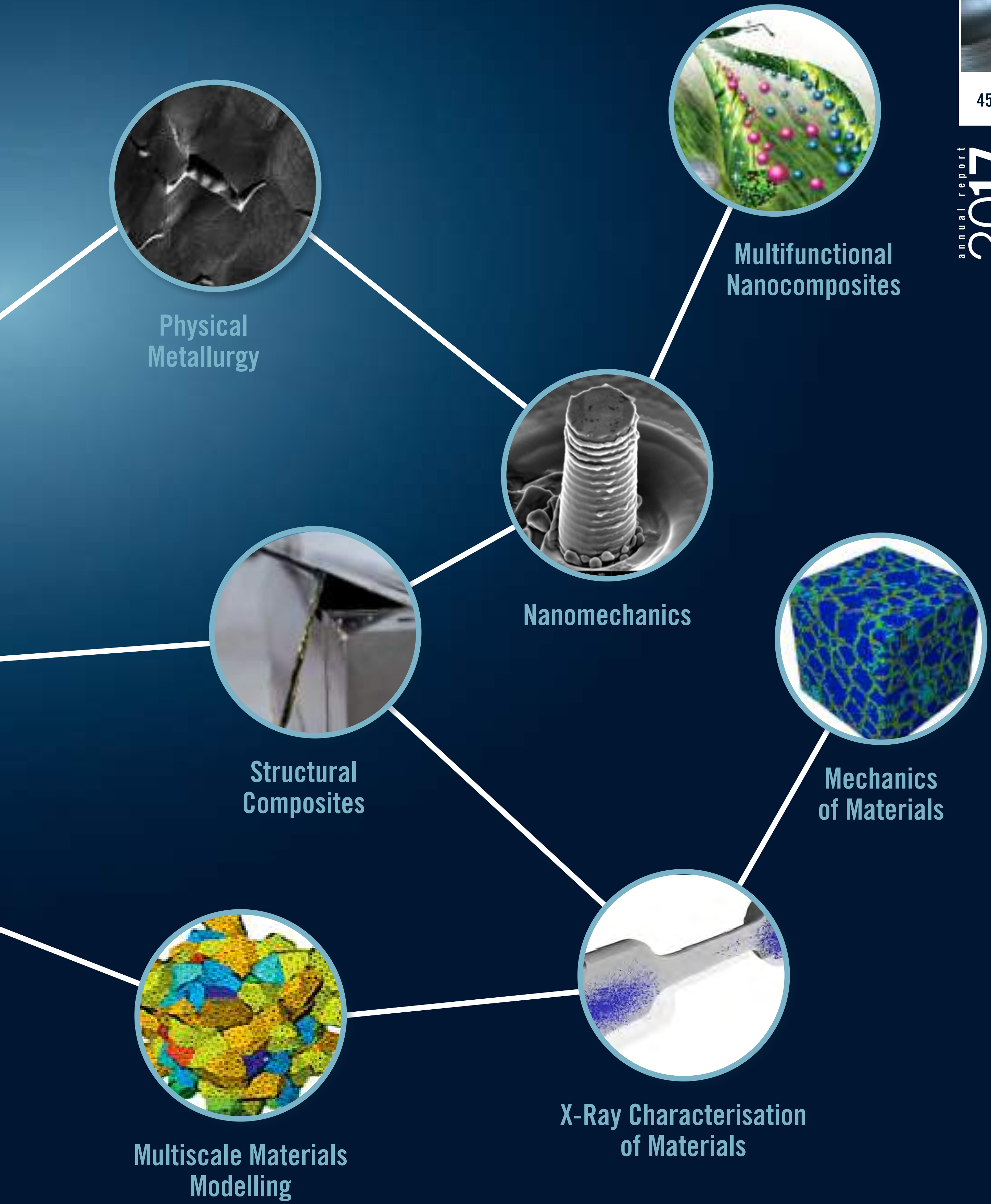
Figure 5. Removal of methoxy groups from the macrocycle molecule on the left leads to the molecule on the right, which forms stable carbon nanotube analogue crystals.

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.**


Physical Metallurgy
Multifunctional Nanocomposites
Nanomechanics
Structural Composites
Mechanics of Materials
Multiscale Materials Modelling
X-Ray Characterisation of Materials

Main research lines

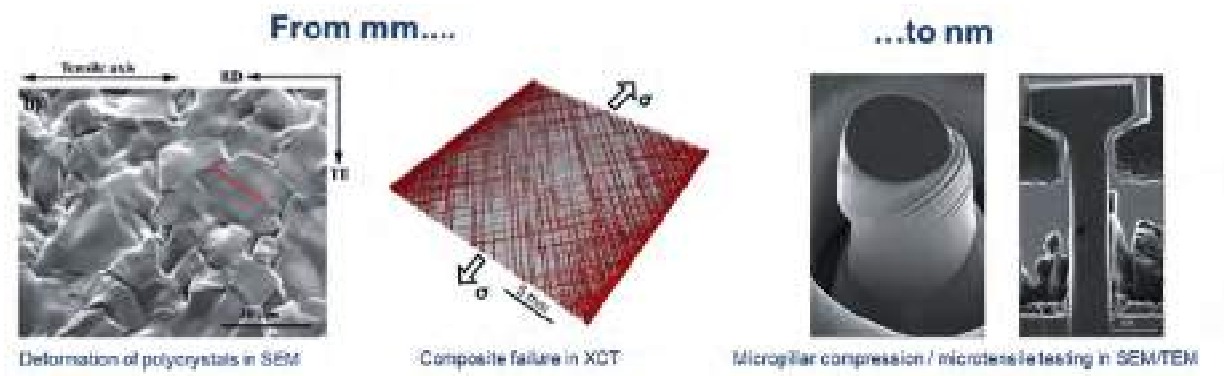
3D characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques:

- 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.

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

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.



Cross-correlation between experiments and multiscale simulations (ICME)

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.

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

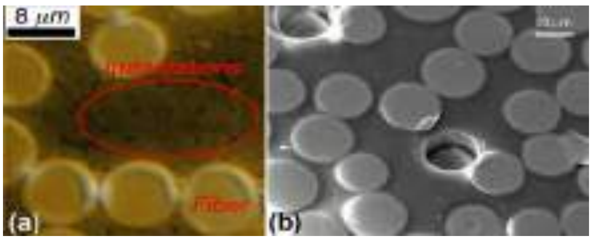


Figure 2. Micromechanical tests to apply at impact conditions: (a) Indentations made on a cross-section of a CFRP. (b) pushed-out debonded fiber.

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 Entwicklungsgeselschaft, 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.

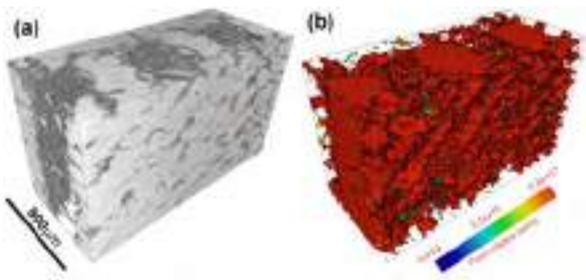
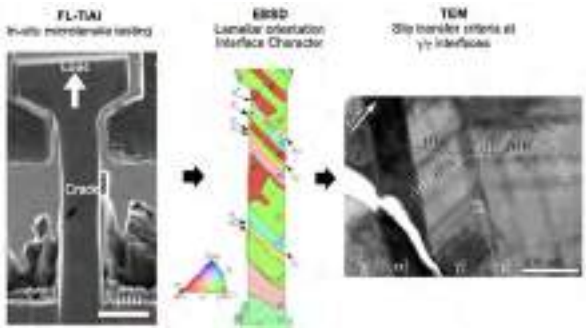


Figure 3. Porous iron preforms used for Al and Al alloy melt infiltration (a) XCT volume of SLM sample. (b)) porosity evaluation of the respective preforms.

Slip transfer across γ-TiAl lamellae in tension

Gamma (γ) 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%) TiB2 (Ti4522XD) alloy, buy combining in-situ microtensile testing, EBSD and TEM.



Reference: A. Palomares, T. Perez-Prado, J. M. Molina-Aldareguia, Materials & Design 146, 2018.

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.

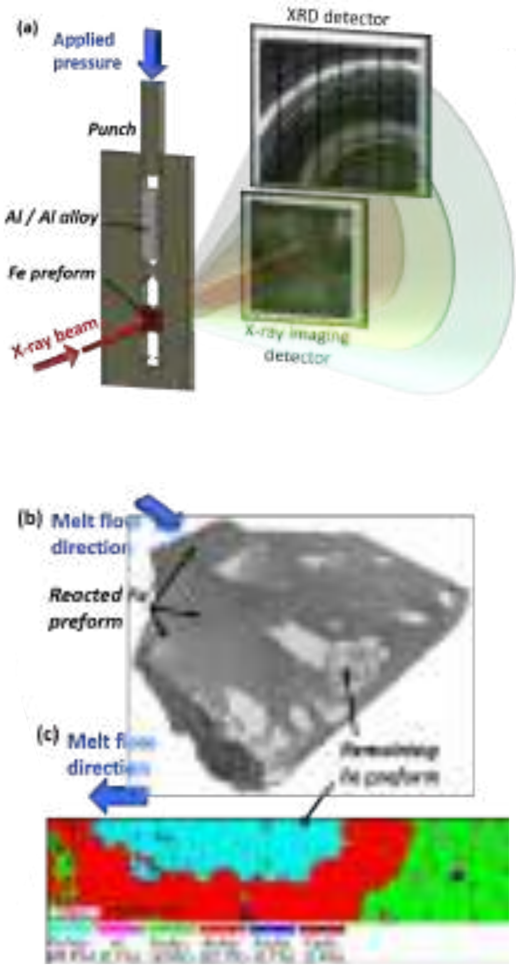


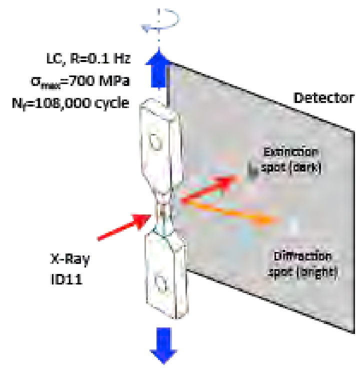
Figure 4. (a) Scheme of the experiment set up at a synchrotron beamline. (b) XCT of the reacted preform after infiltration. (c) EBSD map of the same reacted preform showing the different phases formed during reactive infiltration.

Fatigue crack initiation and propagation studies in Ni superalloys

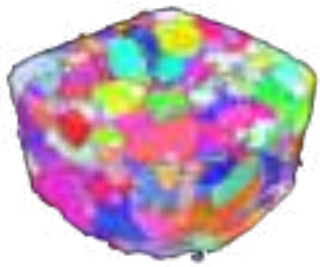
The fatigue growth of microstructural short cracks is an area that remains relatively unexplored. Thus, the development of novel experimental tests to develop a better understanding of the mechanisms involved in the nucleation and propagation of short cracks is crucial, especially to develop predictive 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 speciments. 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.

(a)



(b)



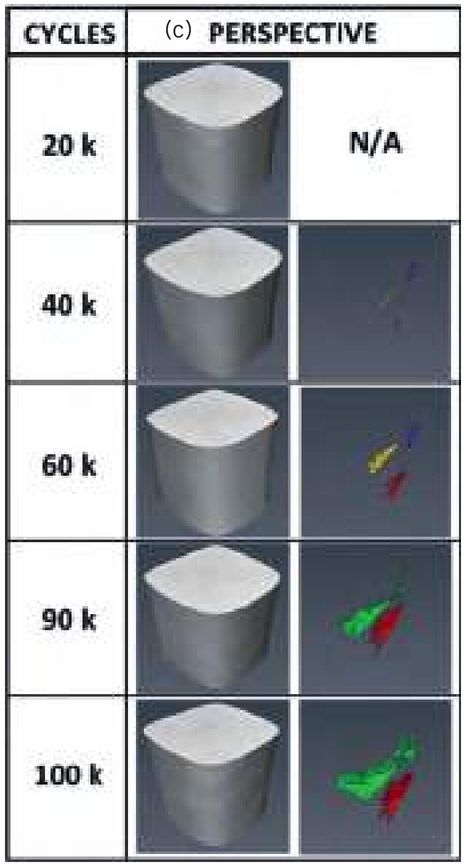


Figure 5. (a) Scheme of the experiment set up at a synchrotron beamline. (b) Initial grain structure by DCT in the gauge length and (c) Crack evolution with number of fatigue cycles determined by PCT.

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.

strategic emerging technologies

Towards fire-safe structural batteries

Electrification of transport.

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.

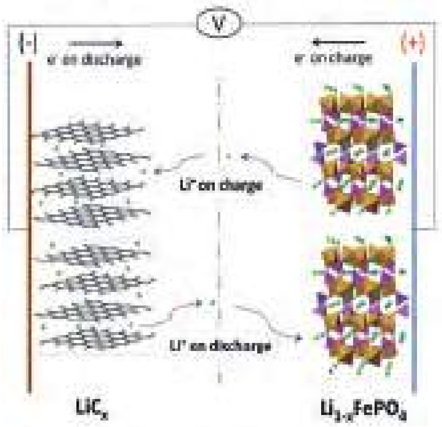


Figure 1. Scheme of a battery operation.

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

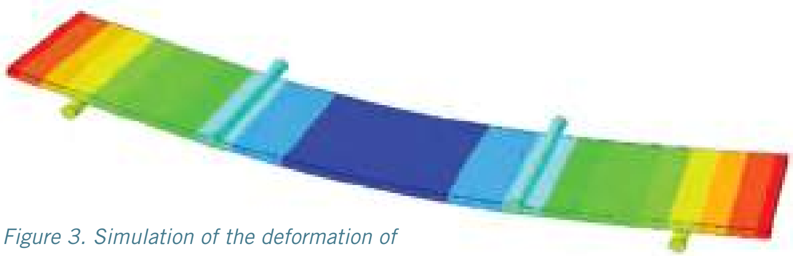
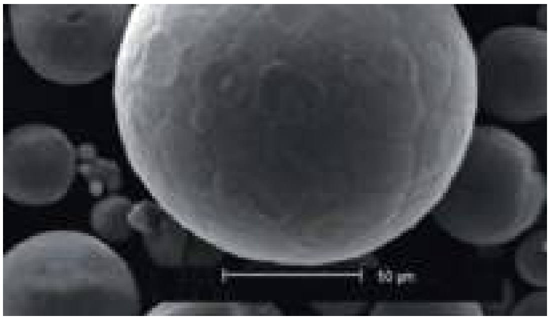


Figure 3. Simulation of the deformation of an energy-storing laminated structure.

Damage-tolerant additive manufacturing of metallic alloys



SEM image of a Mg particle produced by gas atomisation.

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.

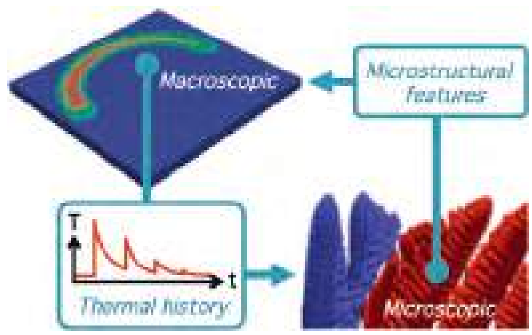


Figure 6. Multiscale modelling strategy of SLM processing.

Simulation-based smart manufacturing of composites

Industry 4.0 (www.en.wikipedia.org/wiki).

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.

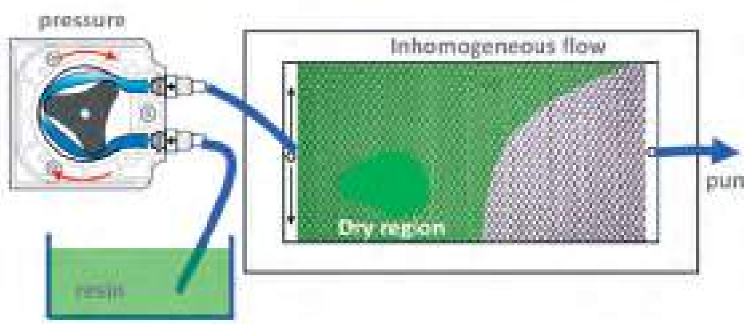


Figure 7. Sketch of a typical resin injection process RTM. Resin inhomogeneous flow is produced as a consequence of manufacturing disturbances that induce the formation of defect in the composite part.

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

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

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

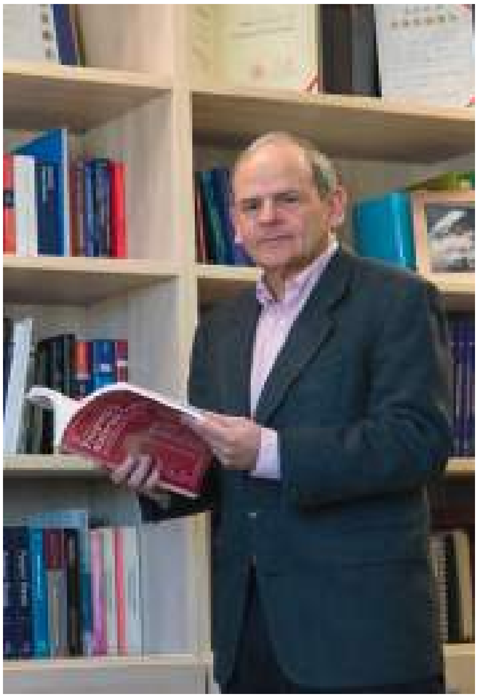
Dr. María Teresa Pérez-Prado

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, charactersation 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. 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 highperformance 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. 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. 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. 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. Ilchat Sabirov

Senior Researcher, Physical Simulation

Ph.D. in Metallurgy from Montanuniversitaet Leoben. Austria

Research Interests

Physical simulation of metallurgical processes, their optimization and study of their effect on the microstructure and properties of metallic materials. Development of novel tools for physical simulation of emerging manufacturing processes. Development of unique thermo-mechanical processing routes that optimise performance of metallic materials.

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. 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); nonequilibirum solidification; directional solidification experiments; in situ imaging of metals and alloys.

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-O_2 batteries.

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.

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.

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.

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. 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.

annex

annex

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

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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
Partners: National Technical University of Athens (Coordinator), Elastotec GmbH Elastomertechniken, Kochanek Entwicklungsgesellschaft, Technica Univerzita V Liberci, Access e.V., Open Source Management Limited, CES Operations AS, Freni BREMBO Spa, Yunzhnoye Design Office named after Mikhail Yangel, IMDEA Materials Institute
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 Aactions
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
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy, Industry and Competitiveness (MEIC) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges 2016
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
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy, Industry and Competitiveness (MEIC) - European Union/Horizon 2020 Programme – M-ERA.NET 2/ International Joint Actions 2017
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
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Collaboration Challenges 2016
Principal Investigator: Prof. Carlos González

Title/Acronym: Advanced materials and nanomaterials Spanish technological platform/ MATERPLAT
Partners: IMDEA Materials Institute (Technical Secretariat)
Period: 2016 – 2018
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy, Industry and Competitiveness (MEIC) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Technological Platforms 2016
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: S 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 atraction. Modality 1
Principal Investigator: Dr. Ruben D. Costa

Title/Acronym: The next generation of rechargeable Li-O_2 batteries
Partners: IMDEA Materials Institute
Period: 2017 – 2021
Funding Institution/Programme: Madrid Regional Government/Grant for research talent atraction. 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 atraction. 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 atraction. 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

Title/Acronym: Modular concept for ultralight removable advanced car seat/ADVANSEAT
Company: Grupo Antolín
Period: 2015 – 2018
Principal Investigators: Prof. Carlos González and Dr. Cláudio S. Lopes

Title/Acronym: Development of new structural materials for energy harvesting and storage/DESMAN
Company: B/E AEROSPACE
Partners: IMDEA Materials Institute (coordinator) and IMDEA Energy Institute
Period: 2014 – 2017
Principal Investigator: Dr. Juan José Vilatela

Title/Acronym: Development and validation of simulation methods for ice and bird ingestion in plane engines/SIMUFOING
Company: ITP Aero
Period: 2014 – 2017
Principal Investigator: Prof. Ignacio Romero

Title/Acronym: Multiscale virtual testing of CFRP samples/VIRTEST
Company: Fokker Aerostructures B.V.
Period: 2014 – 2018
Principal Investigator: Dr. Cláudio S. Lopes

Title/Acronym: Online NDT RTM inspection in composites/ONLINE RTM
Company: AIRBUS Operations S.L.
Period: 2014 – 2018
Principal Investigator: Prof. Carlos González

Title/Acronym: A study of the factors influencing air removal in out-of-autoclave processing of composites/AROOA
Partners: HEXCEL Composites
Period: 2014 – 2017
Principal Investigators: Dr. Federico Sket and Prof. Carlos González

Title/Acronym: Structural analysis of the iter pre-compression rings/ITER PCRs
Company: AIRBUS Defence & Space
Period: 2012 – 2018
Principal Investigator: Prof. Carlos González

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: 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*
Period: 2014-2017
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

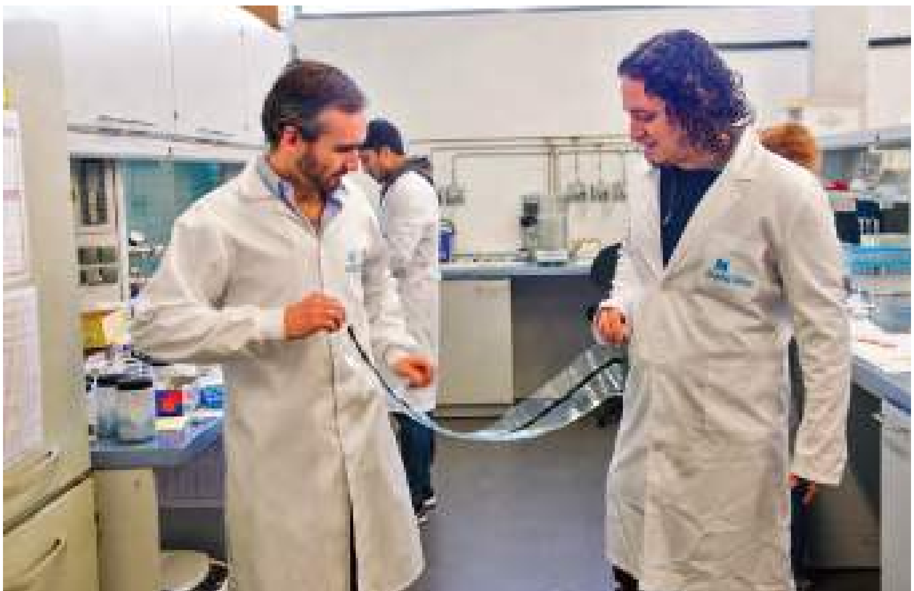
Programme: *China Scholarship Council fellowships*
Project: High strain rate mechanical behavior of advanced high strength steels
Period: 2016-2020
Funding Institution: *China Scholarship Council*
X. Peikang

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: 2015-2019
Funding Institution: *Spanish Ministry of Economy and Competitiveness*
Dr. C. Lopes

Programme: *Ramon y Cajal*
Period: 2013-2018
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: *Postdoctoral Fellowship*
Period: 2017-2019
Funding Institution: *Spanish Ministry of Economy and Competitiveness*
Dr. V. Etacheri

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

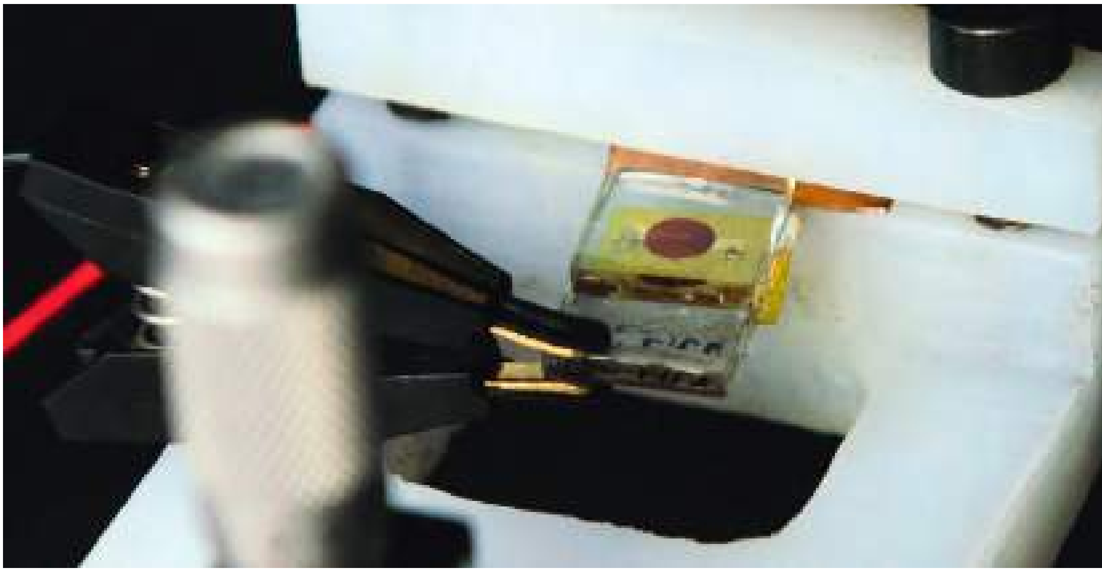
Programme: *Youth Employment Programme / Research assistants and laboratory technicians*
Period: 2017-2019
Funding Institution: *Madrid Regional Government*
A. Martín

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

1. M. A. Monclús, M. Callisti, T. Polcar, L. W. Yang, J. LLorca, and J. M. Molina-Aldareguia. *Selective oxidation-induced strengthening of Zr/Nb nanoscale multilayers*. **Acta Materialia 122**, 1-10, 2017.
2. G. Vallés, M. Panizo-Laiz, C. González, I. Martín-Bragado, R. González-Arrabal, N. Gordillo, R. Iglesias, C. L. Guerrero, J. M. Perlado, and A. Rivera. *Influence of grain boundaries on the radiation-induced defects and hydrogen in nanostructured and coarse-grained tungsten*. **Acta Materialia 122**, 277-286, 2017.
3. A. J. Palomares-García, M. T. Pérez-Prado, and J. M. Molina-Aldareguia. *Effect of lamellar orientation on the strength and operating deformation mechanisms of fully lamellar TiAl alloys determined by micropillar compression*. **Acta Materialia 123**, 102-114, 2017.
4. C. M. Cepeda-Jiménez, J. I. Beltrán, A. Hernando, M. A. García, F. Yndurain, A. Zhilyaev, and M. T. Pérez-Prado. *Tuning the magnetic properties of pure hafnium by high pressure torsion*. **Acta Materialia 123**, 206-213, 2017.
5. P. Hidalgo-Manrique, J. D. Robson, and M. T. Pérez-Prado. *Precipitation strengthening and reversed yield stress asymmetry in Mg alloys containing rare-earth elements: A quantitative study*. **Acta Materialia 124**, 456-467, 2017.
6. H. Liu, B. Bellón, and J. LLorca. *Multiscale modelling of the morphology and spatial distribution of theta' precipitates in Al-Cu alloys*. **Acta Materialia 132**, 611-626, 2017.
7. S-M. Hong, V. Etacheri, C. N. Hong, S. W. Choi, K. B. Lee, and V. G. Pol. *Enhanced Lithium and Sodium-Ion storage in an interconnected Carbon network comprising electronegative Fluorine*. **ACS Applied Materials & Interfaces 9**, 18790-18798, 2017.
8. B. M. D. Puscher, M. F. Aygueler, P. Docampo, and R. D. Costa. *Unveiling the dynamic processes in hybrid Lead Bromide Perovskite nanoparticle thin film devices*. **Advanced Energy Materials 7**, 2017.
9. D. Portillo, D. del Pozo, D. Rodríguez-Galán, J. Segurado, and I. Romero. *MUESLI - a Material UnivErSal LIbrary*. **Advances in Engineering Software 105**, 1-8, 2017.
10. A. Lennert, M. Sternberg, K. Meyer, R. D. Costa, and D. M. Guldi. *Iodine-pseudohalogen ionic liquid-based electrolytes for quasi-solid-state dye-sensitized solar cells*. **ACS Applied Materials & Interfaces 9**, 33437-33445, 2017.
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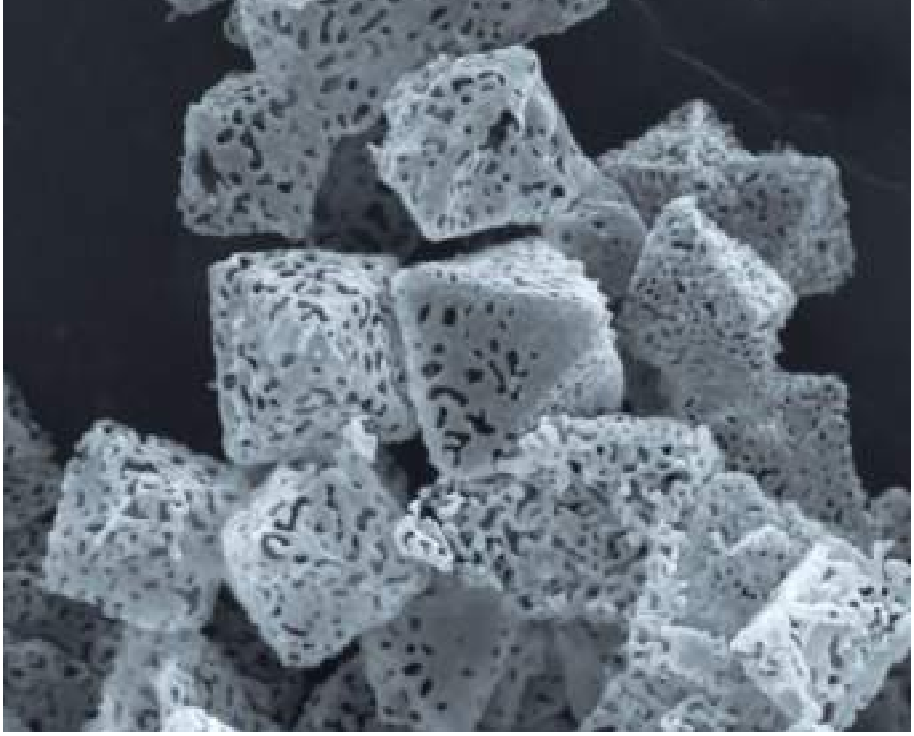

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3.3. Book Chapters

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3.4. Patent Applications

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3.5. International Conferences

Invited and Plenary talks

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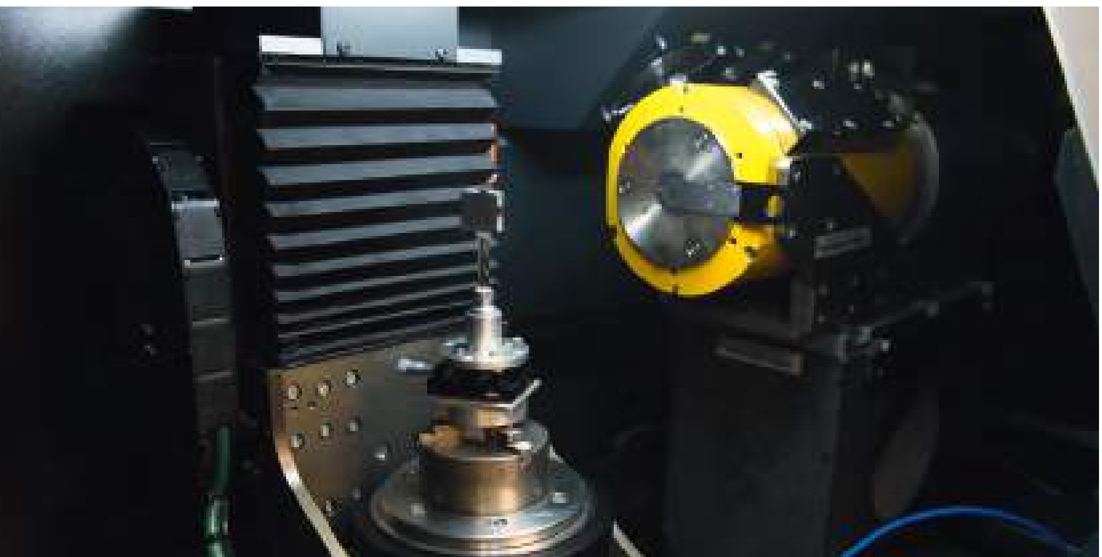
2. *"Optimum layer thickness for high temperature mechanical properties of ARB Cu/Nb nanoscale multilayers"*, J. M. Molina-Aldareguia, J. Snel, M. Monclús, N. Mara, I. Beyerlein, J. LLorca, **TMS 146th Annual Meeting and Exhibition (TMS 2017)**, San Diego, USA, February – March 2017.
3. *"Fracture toughness of Al/SiC nanolaminates: Experiments and simulations"*, C. Mayer, L. W. Yang, V. Carollo, J. K. Baldwin, N. Mara, J. M. Molina-Aldareguia, N. Chawla, **TMS 146th Annual Meeting and Exhibition (TMS 2017)**, San Diego, USA, February – March 2017.
4. *"Micro and nanomechanical testing as a useful tool to enable fast and efficient design of structural materials"*, J. M. Molina-Aldareguia, **European Nanomechanical Testing Conference 2017 (Nanobrücken 2017)**, Manchester, United Kingdom, April 2017.
5. *"Microstructure based modeling of fatigue life in Inconel 718"*, J. Segurado, **International Workshop on Quantitative Mechanistic Nucleation and Microstructure-sensitive Growth of Fatigue Cracks**, Oxford University, United Kingdom, April 2017.
6. *"A roadmap for virtual design of metallic materials: from atoms to components"*, J. LLorca, **Res Metallica Symposium**, Katolieke University of Leuven, Leuven, Belgium, May 2017.
7. *"A multiscale modelling roadmap for virtual processing and virtual testing of metallic materials*", J. LLorca, **29th Canadian Materials Science Conference**, Ottawa, Canada, June 2017.
8. *"Functional LDH: a new nanomaterial to flame retardant polymers"*, D.-Y. Wang, **Polymer Processing Society (PPS)**, Dresden, Germany, June 2017.



9. *"CNT fibre composites"*, J. J. Vilatela, **Polymer Processing Society (PPS)**, Dresden, Germany, June 2017.
10. *"High-throughput methods for accelerated materials development"*, S. Milenkovic, **3rd Metallurgical & Materials Engineering Congress of South-East Europe (MME-SEE)**, Belgrade, Serbia, June 2017.
11. *"Nuevos algoritmos para el diseño/cálculo de estructuras aeronáuticas"*, C. González, **Innovación en estructuras de materiales compuestos, Cursos de Verano de la Universidad Internacional Menéndez Pelayo**, Santander, Spain, June 2017.
12. *"Functionalization of nanomaterials: A new way to flame retardant polymers"*, D.-Y. Wang, **8th Asia-Europe Symposium on Processing and Properties of Reinforced Polymers (AESP8)**, Chengdu, China, June – July 2017.
13. *"On the effect of grain size on the strength of FCC polycrystals: a multiscale approach"*, S. Hauoala, J. Segurado, J. LLorca, **54th Annual Technical Meeting, Society of Engineering Science (SES)**, Boston, Massachusetts, USA, July 2017.
14. *"Microstructure-based modeling of the fatigue performance of metallic alloys: current status and challenges"*, A. Cruzado, M. Jiménez, S. Lucarini, J. Segurado, J. M. Molina-Aldareguía, J. LLorca, **IUTAM Symposium on Multi-scale Fatigue, Fracture & Damage of Materials in Harsh Environments**, Galway, Ireland, August 2017.
15. *"Bio-rubber coatings for single-point light-emitting diodes and displays"*, R. D. Costa, **IUPAC International Symposium on MacroMolecular Complexes (MMC-17)**, Tokyo, Japan, August 2017.
16. *"General energy-entropy-momentum integration methods for non-linear themomechanics"*, I. Romero, D. Portillo, **3rd International Conference on Multiscale Computational Methods for Solids and Fluids**, Ljubljana, Slovenia, September 2017.
17. *"An analysis of the influence of grain size on the strength of FCC polycrystals by means of computational homogenization"*, S. Haouala, J. Segurado, J. LLorca, **Session on Size Effects on Metal Plasticity, XIV International conference on Computational Plasticity (COMPLAS 2017)**, Barcelona, Spain, September 2017.
18. *"Grain size effects in polycrystalline homogenization: strain gradient and mean-free path contributions"*, J. Segurado, D. Rodríguez, S. Haouala, I. Romero, J. LLorca, **Session on Size Effects on Metal Plasticity, XIV International conference on Computational Plasticity (COMPLAS 2017)**, Barcelona, Spain, September 2017.
19. *"Precipitate strengthening of Al-Cu alloys: A multiscale dislocation dynamics approach"*, R. Santos, G. Esteban, E. Martínez, L. Capolungo, J. Segurado, J. LLorca, **Session on Computational Multiescale Plasticity, XIV International conference on Computational Plasticity (COMPLAS 2017)**, Barcelona, Spain, September 2017.
20. *"Multiscale modelling of plasticity: towards virtual tests of metallic materials"*, J. LLorca, **XIV International conference on Computational Plasticity (COMPLAS 2017)**, Barcelona, Spain, September 2017.
21. *"Anisotropy of mechanical and functional properties in SPD processed metallic materials"*, I. Sabirov, **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2017)**, Thessaloniki, Greece, September 2017.

22. *“High throughput investigation of solute effects in beta titanium alloys”*, S. Milenkovic, Y. Cui, C. Wang, M. T. Pérez-Prado, **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2017)**, Thessaloniki, Greece, September 2017.
23. *“Hybrid nanocarbon-based and bio-related materials for optoelectronic devices”*, R. D. Costa, **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2017)**, Thessaloniki, Greece, September 2017.
24. *“Design and fabrication of AM metallic powders at the lab scale”*, M. T. Pérez-Prado, **Alloys for Additive Manufacturing Symposium (AAMS17)**, Empa, Dübendorf, Switzerland, September 2017.
25. *“Integration of multiscale experiments & multiscale materials models: the path towards virtual testing”*, J. LLorca, **2017 Materials Research and Data Science (MRaDS) Conference**, Rockville, Maryland, USA, September 2017.
26. *“Multiscale virtual structural testing: Towards simulation-based design and certification of aircraft structures”*, C. S. Lopes, C. González, **6th Challenges in European Aerospace (CEAS) Air & Space Conference**, Invited in representation of EUROMECH, Bucharest, Romania, October 2017.
27. *“Molecular design and functionalization of nano-hybrid: an important way to new generation flame retardant”*, D.-Y. Wang, **2nd Asia-Oceania Symposium for Fire Safety Materials Science and Engineering (AOFSM 2017)**, Shenzhen, China, October 2017.
28. *“CNT fibre/semiconductor hybrids”*, J. J. Vilatela, **Physics Engineering Congress UIA**, Mexico City, Mexico, November 2017.
29. *“Influence of the grain boundary networks and triple junctions on the deformation mechanisms in magnesium”*, C. M. Cepeda-Jiménez, **Materials Research Society Fall Meeting (2017 MRS Fall Meeting)**, Boston, Massachusetts, USA, November – December 2017.
30. *“Understanding the Role of Interfaces on Fully Lamellar TiAl Alloys through Micromechanical Testing”*, J. Molina-Aldareguia, A. Palomares, M. T. Pérez-Prado, **Materials Research Society Fall Meeting (2017 MRS Fall Meeting)**, Boston, Massachusetts, USA, November – December 2017.

Regular Contributions

1. *“Hybrid nanocarbon-based and bio-related materials for optoelectronic devices“*, R. D. Costa, **AP-HOPV**, Yokohama, Japan, February 2017.
2. *“Extraction of Crystal Plasticity Parameters of IN718 Using High Temperature Microcompression”*, B. Gan, A. Cruzado, M. Jiménez, K. Ostolaza, A. Linaza, J. Segurado, J. LLorca, J. M. Molina-Aldareguia, **TMS 146th Annual Meeting and Exhibition (TMS 2017)**, San Diego, USA, February – March 2017.
3. “Analysis of the damage evolution in steel specimens under tension by means of XRCT”, F. Suarez, J. C. Gálvez, D. A. Cendón, J. M. Atienza, F. Sket, J. M. Molina-

Aldareguia, **International Symposium on Notch Fracture (ISNF)**, Santander, Spain, March 2017.

4. *"CNT fibres for energy management"*, J. J. Vilatela, **5th International Conference on Multifunctional, Hybrid and Nanomaterials**, Lisbon, Portugal, March 2017.
5. *"Microscale testing techniques for constituent characterization in computational micromechanics"*, F. Naya, M. Monclús, J. M. Molina-Aldareguia, C. S. Lopes, C. González, **CompTest 2017**, Leuven, Belgium, April 2017.
6. *"Atomistic simulations of dislocation/precipitate interactions in Mg-Al alloys"*, A. Moitra, J. Segurado, J. LLorca, **MRS Spring Meeting**, Phoenix, Arizona, USA, April 2017.
7. *"Phase field modelling of θ' precipitation during aging of Al-4wt.%Cu alloys: a multiscale approach"*, H. Liu, G. Esteban-Manzanares, B. Bellón, I. Sabirov, J. LLorca, **MRS Spring Meeting**, Phoenix, Arizona, USA, April 2017.
8. *"Selective oxidation-induced strengthening of Zr/Nb nanoscale multilayers interactions in Mg-Al alloys"*, M. A. Monclús, L. W. Yang, M. Callisti, T. Polcar, J. M. Molina-Aldareguia, J. LLorca, **MRS Spring Meeting**, Phoenix, Arizona, USA, April 2017.
9. *"MUESLI: a Material UnivErSal Library"*, I. Romero, D. Portillo, D. Rodríguez-Galán, J. Segurado, D. del Pozo, **4th World Congress on Integrated Computational Materials Engineering (ICME2017)**, Ypsilanti, Michigan, USA, May 2017.
10. *"Mutiscale modelling of θ' precipitation during aging of Al-4wt.%Cu alloys"*, H. Liu, G. Esteban-Manzanares, B. Bellón, I. Sabirov, J. LLorca, **4th World Congress on Integrated Computational Materials Engineering (ICME2017)**, Ypsilanti, Michigan, USA, May 2017.
11. *"A microlevel capillary study in composite materials by X-ray tomography"*, J. Castro, F. Sket, C. González. **Congreso Bienal De Materiales Compuestos (MATCOMP17)**, San Sebastian, Spain, June 2017.
12. *"Mechanisms of air removal and void development in Out-of-Autoclave processing of laminates"*, J. J. Torres, F. Sket, C. González, M. Simmons, **Congreso Bienal De Materiales Compuestos (MATCOMP17)**, San Sebastian, Spain, June 2017.
13. *"Obtención de fibra de carbono reciclada mediante pirolisis de preimpregnados curados"*, A. Fernández Gorgojo, C. S. Lopes, R. Guzmán, C. González, F. A. López, **Congreso Bienal De Materiales Compuestos (MATCOMP17)**, San Sebastián, España, June 2017.
14. *"Multifunctional composites based on CNT fibres"*, J. J. Vilatela, **Congreso Bienal De Materiales Compuestos (MATCOMP17)**, San Sebastián, Spain, June 2017.
15. *"Bottom-up multiscale approach on transverse cracking of cross-ply laminates"*, M. Herráez, C. Gonzalez, C. S. Lopes, **International Conference on Computational Fracture and Failure of Materials and Structures (CFRAC 2017)**, Nantes, France, June 2017.
16. *"Grain orientation effects and void growth in titanium: three-dimensional experiments and crystal plasticity simulations"*, M. Pushkareva, F. Sket, J. Segurado, J. LLorca, M. Yandouzi, A. Weck, **29th Canadian Materials Science Conference**, Ottawa, Canada, June 2017.

17. *"Hierarchical engineering of halloysite nanotubeand its enhancement in fire safety and mechanical property of epoxy resin"*, Z. Li, D.-Y. Wang, **Polymer Processing Society 2017 (PPS2017)**, Dresden, Germany, June 2017.
18. *"Uncertainty quantification in the dynamic response of assembled structures"*, E. Menga, C. López, S. Hernández, I. Romero, M. Sánchez-Naranjo, **International Forum on Aeroelasticity and Structural Dynamics**, Como, Italy, June 2017.
19. *"Variational methods for coupling nonlinear beams and continua"*, I. Romero, **VII International Conference on Coupled Problems in Science and Engineering**, Rhodes, Greece, June 2017.
20. *"Energy-Entropy-Momentum integration schemes"*, D. Portillo, I. Romero, **Congreso de Métodos Numéricos en Ingeniería 2017**, Valencia, Spain, July, 2017.
21. *"MUESLI: a Material UnivErSal Library"*, E. M. Andrés, D. del Pozo, D. Rodriguez, D. Portillo, J. Segurado, I. Romero, **Congreso de Métodos Numéricos en Ingeniería 2017**, Valencia, Spain, July 2017.
22. *"Algorithms for the integration of non-smooth elasto-visco-plastic models"*, D. del Pozo, I. Romero, **Congreso de Métodos Numéricos en Ingeniería 2017**, Valencia, Spain, July 2017.
23. *"Development of a thermoθmechanically coupled crystal plasticity finite element modeling framework"*, J. Li, J. Segurado, I. Romero, **Congreso de Métodos Numéricos en Ingeniería 2017**, Valencia, Spain, July 2017.
24. *"Fast Fourier Transform based homogenization of the cyclic behaviour and fatigue life prediction of polycrystalline superalloys"*, J. Segurado, J. LLorca, A. Cruzado, S. Lucarini, **Congreso Métodos Numéricos en la Ingeniería**, Valencia, Spain, July 2017.
25. *"Micromechanical model for the simulation of creep deformation in Inconel 718"*, E. M. Andrés, J. Segurado, I. Romero, **Congreso de Métodos Numéricos en Ingeniería 2017**, Valencia, Spain, July 2017.
26. *"Functionalization of nanomaterials vs time to ignition of polymeric materials"*, S. Hu, D.-Y. Wang, **Fire Retardant Polymeric Material 2017 (FRPM17)**, Manchester, United Kingdom, July 2017.
27. *"Additive alloy melting: A novel high-throughput method for accelerated alloy fabrication"*, S. Milenkovic, M. Cristobal, D. San Martin, C. Capdevila, **6th Decennial International Conference on Solidification Processing**, Old Windsor, United Kingdom, July 2017.
28. *"Pressureless reactive infiltration of liquid Al into porous Fe preforms"*, S. Milenkovic, A. Hynowska, **6th Decennial International Conference on Solidification Processing**, Old Windsor, United Kingdom, July 2017.
29. *"Ballistic performance of needle-punched nonwoven fabrics: experiments and simulations"*, F. Martínez-Hergueta, A. Ridruejo, C. González, J. LLorca, **54th Annual Technical Meeting, Society of Engineering Science**, Boston, Massachusetts, USA, July 2017.
30. *"Modeling of fatigue fracture of Inconel 718 by means of crystal plastic and computational homogenization"*, J. Segurado, A. Cruzado, S. Lucarini, J. LLorca,

54th Annual Technical Meeting, Society of Engineering Science, Boston, Massachusetts, USA, July 2017.

31. *"Strengthening of Mg-Al alloys by precipitates: An atomistic analysis"*, A. Moitra, J. LLorca, **54th Annual Technical Meeting, Society of Engineering Science**, Boston, Massachusetts, USA, July 2017.
32. *"Phase behaviour of annealed CNT Fibers/PVDF composites studied by X-Ray diffraction"*, J. P. Fernández-Blázquez, A. Monreal-Bernal, J. J. Vilatela, **European Polymer Federation (EPF 2017)**, Lyon, France, July 2017.
33. *"A virtual testing approach to materials selection for impact shielding applications"*, D. Garijo, C. S. Lopes, O. Falcó, C. González, V. Votsios, **21st International Conference on Composite Materials (ICCM-21)**, Xi'an, China, August 2017.
34. *"Fibre kinking: from micro to mesomechanics"*, M. Herráez, C. González, C. S. Lopes, **6th ECCOMAS Thematic Conference on the Mechanical Response of Composites** (**Composites 2017)**, Eindhoven, The Netherlands, September 2017.
35. *"A multi-material shell modelling of mechanical behaviour of triaxial braided composites"*, A. García-Carpintero, C. S. Lopes, M. Herráez, J. Xu, C. González, **6th ECCOMAS Thematic Conference on the Mechanical Response of Composites** (**Composites 2017)**, Eindhoven, The Netherlands, September 2017.
36. *"Damage and failure of woven composites from a bottom-up multiscale modelling approach"*, J. Múgica, J. Xu, F. Naya, C. S. Lopes, C. González, **6th ECCOMAS Thematic Conference on the Mechanical Response of Composites** (**Composites 2017)**, Eindhoven, The Netherlands, September 2017.
37. *"Fibre kinking: from micro to mesomechanics"*, M. Herráez, C. González, C. S. Lopes, **6th ECCOMAS Thematic Conference on the Mechanical Response of Composites** (**Composites 2017)**, Eindhoven, The Netherlands, September 2017.
38. *"Assessment of eutectic trough and solidification paths in NiAl-Cr-W system"*, S. Milenkovic, A. Varona-Caballero, **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2017)**, Thessaloniki, Greece, September 2017.

39. *"Electrode architectures for enhanced Na-ion battery performance"*, V. Etacheri, **International Conference on Functional Nanomaterials and Nanodevices**, Budapest, Hungary, September 2017.
40. *"Fast Fourier Transform based homogenization of the cyclic behaviour and fatigue life prediction of polycrystalline superalloys"*, J. Segurado, S. Lucarini, **XIV International conference on Computational Plasticity COMPLAS 2017**, Barcelona, Spain, September 2017.
41. *"Grain size effects in polycrystalline homogenization: strain gradient and mean-free path contributions"*, J. Segurado, D. Rodríguez-Galán, S. Haloula, I. Romero, J. LLorca, XI **International Conference on Computational Plasticity, Fundamentals and Applications** (**COMPLAS 2017)**, Barcelona, Spain, September 2017.
42. *"Numerical modeling of of the ballistic behavior of a needlepunched nonwoven"*, F. Martínez-Hergueta, A. Ridruejo, C. González, J. LLorca, **XIV International conference on Computational Plasticity (COMPLAS 2017)**, Barcelona, Spain, September 2017.
43. *"General energy-entropy-momentum integration methods for non-linear themomechanics"*, I. Romero, D. Portillo, **3rd International Conference on Multiscale Computational Methods for Solids and Fluids**, Ljubljana, Slovenia, September 2017.
44. *"Microstructure based modeling of fatigue life in Inconel 718"*, S. Lucarini, J. Segurado, **27th International Workshop on Computational Mechanics of Materials (IWCMM-27)**, Leuven, Belgium, September 2017.
45. *"Thermodynamically consistent integration of discrete thermo-elastoplastic dynamics"*, J. C. García Orden, D. Portillo, I. Romero, **IUTAM Symposium on Intelligent Multibody Systems Dynamics, Control, Simulation**, Sozopol, Bulgaria, September 2017.
46. *"Thermotropic phase behaviour of CNT Fibers/liquid crystal polymer composites"*, C. Sobrino-Verde, V. San Miguel, V. Reguero, J. J. Vilatela, J. P. Fernández-Blázquez, **17th Baltic Polymer Symposium (COST action CA15107)**, Tallinn, Estonia, September 2017.
47. *"Virtual coupon testing: adding value in the aerospace industry"*, B. Tijs, C. S. Lopes, O. Falcó, W. Wilson, M. Markestein, M. Funnell, **6th ECCOMAS Thematic Conference on the Mechanical Response of Composites (Composites 2017)**, Eindhoven, The Netherlands, September 2017.
48. *"Impact of expandable graphite on the flame retardancy and mechanical properties of rigid polyurethane foams with varied density"*, P. Acuña, D.-Y. Wang, **2nd Asia-Oceania Symposium for Fire Safety Materials Science and Engineering (AOFSM 2017)**, Shenzhen, China, October 2017.
49. *"Bio-based composite with good mechanical properties and flame retardancy"*, Y. Yang, D.-Y. Wang, **2nd Asia-Oceania Symposium for Fire Safety Materials Science and Engineering (AOFSM 2017)**, Shenzhen, China, October 2017.
50. *"Field-assisted sintering of WC hardmetals with Cr-based binder"*, X. X. Deng, J. M. Torralba, A. García-Junceda, **Euro PM2017 Congress & Exhibition**, Milan, Italy, October 2017.

51. *"Micromechanics of fully lamellar TiAl alloys"*, J. M. Molina-Aldareguia, A. Palomares, M. T. Pérez-Prado. **Nanomechanical testing in Materials Research and Development VI**, Dubrovnik, Croatia, October 2017.
52. *"Anisotropy and microstructure in 3D printed In 718"*, S. Subedi, A. Palomares, J. M. Molina-Aldareguía, J. LLorca, S. Cong and A. D. Rollett, **18th International Conference on Textures of Materials (ICOTOM 18)**, St. George, Utah, USA, November 2017.
53. *"Effect of austenite fraction on the microstructure and properties of duplex stainless steels consolidated by field-assisted sintering"*, A. García-Junceda, C. Díaz Rivera, V. Gómez Torralba, M. Campos, J. M. Torralba, **International Conference on SINTERING 2017**, California, USA, November 2017.
54. *"Microstructural changes on Co-9Al-9W alloy produced by SPS and Ti and Ta additions"*, M. Cartón-Cordero, M. Campos, J. M. Torralba, **International Conference on SINTERING 2017**, California, USA, November 2017.
55. *"Microstructural evolution in a four group element ODS ferritic steel (Y-Al-Ti-Zr) consolidated by SPS"*, E. Macia, J. Cornide, A. García-Junceda, M. Campos, J. M. Torralba. **International Conference on SINTERING 2017**, California, USA, November 2017.
56. *"Energy storage in structural composites using nanostructured fibres"*, J. J. Vilatela. **Lighter Conference**, Gothenburg, Sweden, November 2017.
57. *"Modelling of the mechanical behaviour of polyurethane foams by means of micromechanical characterization and computational homogenization"*, M. Marvi-Mashhadi, C. S. Lopes, J. LLorca, **Conference on Computational Modeling of Complex Materials across the Scales**, Paris, France, November 2017.
58. *"Deformation mechanism map of Cu/Nb nanoscale metallic multilayers as a function of temperature and layer thickness"*, J. M. Molina-Aldareguia, J. Snel, M. A. Monclús, N. Mara, I. Beyerlein, J. LLorca, **Materials Research Society Fall Meeting (2017 MRS Fall Meeting),** Boston, Massachusetts, USA, November – December 2017.

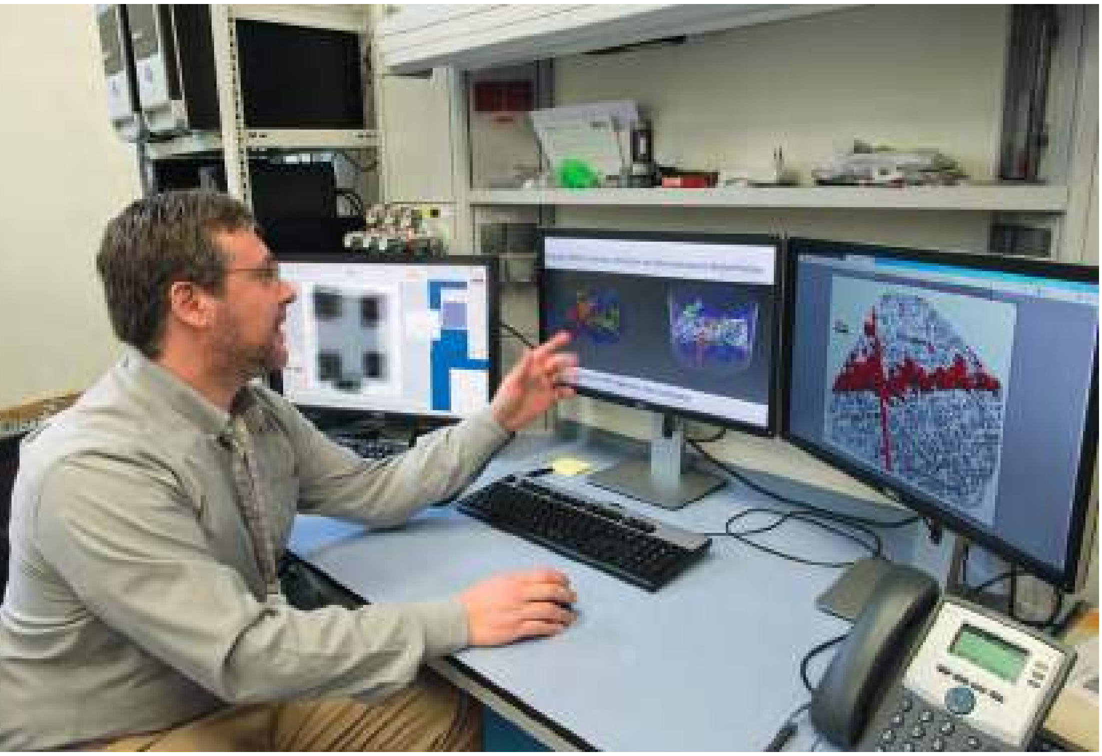
Membership in Organising Committees

1. **TMS 2017: 146th Annual Meeting and Exhibition**. M. T. Pérez-Prado (Symposium organizer). San Diego, USA, March 2017
2. **The Asia-Europe Symposium on Processing and Properties of Reinforced Polymers—AESP2017.** D-Y. Wang (Member of International Advisory Board). Chengdu, China, May 2017.
3. **Summer School on Composite Materials (Dynacomp project)**. F. Sket, J. Molina, C. González (Organizers, Lecturers). IMDEA Materials Institute, Getafe, Spain, July 2017
4. **16th European Meeting on Fire Retardant Polymeric Materials (FRPM2017).** D-Y. Wang (Member of International Scientific Committee). Manchester, UK, July 2017.

5. **Symposium on High Temperature Materials (EUROMAT 2017).** S. Milenkovic (Organizer). Thessaloniki, Greece, September 2017.
6. **The 2nd** Asia-Oceania Symposium on Fire Safety Materials Science and Engineering (AOFSM›2). D-Y. Wang (Member of International Scientific Committee). Shenzhen, China, October 2017.
7. **MRS 2017: Fall Meeting & Exhibit.** M. T. Pérez-Prado (Symposium organizer). Boston, USA, November 2017.
8. **LightMAT 2017, 2nd International Conference on Light Materials – Science and Technology**. M. T. Pérez-Prado (Member of the International Advisory Board). Bremen, Germany, November 2017.

3.6. Hosting and Organisation of International Conferences and Workshops

1. **Summer School on Composite Materials – DYNACOMP Training Network (H2020-Marie Skłodowska-Curie action).** J. M. Molina, C. González, F. Sket and G. Infante, July 2017.
2. **Meeting with Spanish Industry: Presentation of BioLed technology.** R. Costa, M. A. Rodiel in collaboration with smartLIGHTING, November 2017.



3.7. Invited Seminars and Lectures

1. *"A multiscale modelling strategy for virtual design of metallic alloys"*, J. LLorca. Departments of Engineering, **Cambridge University**, Cambridge, United Kingdom, February 2017.
2. *"A multiscale modelling strategy for virtual processing and virtual testing of metallic alloys"*, J. LLorca. Departments of Materials and Mechanical Engineering, **Imperial College**, London, United Kingdom, February 2017.
3. *"Multiscale modelling strategies for virtual processing and virtual testing of metallic alloys"*, J. LLorca, **Brunel Centre for Advanced Solidification Technology, Brunel University**, Uxbridge, United Kingdom, February 2017.
4. *"New approaches for lighting applications"*, R. D. Costa, **JX Company**, Yokohama, Japan, February 2017.
5. *"New approaches for lighting applications"*, R. D. Costa, **University of Waseda**, Tokyo, Japan, February 2017.
6. *"Multiscale design and simulation of composites at IMDEA Materials"*, C. S. Lopes, **INEGI-Institute of Science and Innovation in Mechanical and Industrial Engineering**, Porto, Portugal, February 2, 2017.
7. *"A multiscale modelling trategy for virtual processing and virtual testing of metallic alloys"*, J. LLorca, **Institute of Mechanics, Materials and Civil Engineering, Université Catholique de Louvain**, Louvain le Neuve, Belgium, March 2017.
8. *"Computational and data-driven discovery of materials"*, M. Haranczyk, École **Polytechnique Fédérale de Lausanne (EPFL)**, Lausanne , Switzerland, March 2017"
9. *"A roadmap for virtual design of metallic materials: from atoms to components"*, J. LLorca, **Center for 4D Materials Science, Arizona State University**, Tempe, Arizona, USA, April 2017.
10. *"Microstructure based simulations of a polycrystalline Ni superalloy"*, J. Segurado, **Oxford University**, Oxford, United Kingdom, April 2017.
11. *"A roadmap for virtual design of metallic materials: from atoms to components"*, J. LLorca, **Computational Mechanics Research Laboratory, John Hopkins University**, Baltimore, Maryland, USA, May 2017.
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.
13. *"CNT fibres for energy managing devices"*, J. J. Vilatela, **Nanofabrication Centre, Instituto Politécnico Nacional (IPN)**, Mexico City, Mexico, May 2017.
14. *"Microscale & mesocale characterisation of composites: towards a bottom-up design approach"*, J. LLorca, **Center for Composite Materials, University of Delaware**, Newark, Delaware, USA, May 2017.
15. *"Multiscale modeling of the mechanical behavior of polyurethane foams"*, J. LLorca, **Advanced Materials & Systems Research, BASF**, Wyandotte, Michigan, USA, May 2017.

16. *"The concept of Lify"*, R. D. Costa, **Transforming mobility, AUDI Summit**, Barcelona, Spain, 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.
18. *"Multiscale modelling of precipitation hardening in Al and Mg alloys"*, J. LLorca, **School of Civil and Environmental Engineering, Cornell University**, Ithaca, New York, USA, July 2017.
19. *"The controversial microplasticity of polycrystalline Magnesium"*, M. T. Pérez-Prado, **Xi´an Jiao Tong University**, Xi´an, China, July 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.
23. *"The future of the lighting"*, R. D. Costa, **Emtech**, Paris, France, September 2017.
24. *"Novel approaches in thin-films lighting technologies"*, R. D. Costa, **University of Crete**, Crete, Greece, September 2017.
25. *"Design and fabrication of additive manufacturing metallic powders at the lab scale"*, M. T. Pérez-Prado, **Universidad Politécnica de Cataluña**, Barcelona, Spain, October 2017.
26. *"In-situ mechanical charactarization of materials with X-ray tomography"*, F. Sket, **German Aerospace Center (DLR) Department of Metals and Hybrid Materials**, Cologne, Germany, October 2017.
27. *"A magic macromolecular world"*, D.-Y. Wang, **Beijing Institute of Fashion Technology**, Beijing, China, October 2017.
28. *"Layer double hydroxide (LDH) based polymer nanocomposites: Functionalization vs Flammability"*, D.-Y. Wang, **South China University of Science and Technology**, Shenzhen Shi, China, October 2017.
29. *"New generation nano flame retardant materials"*, D.-Y. Wang, **Shenyang University of Chemical Technology**, Shenyang, China, October 2017.
30. *"New generation of flame retardant materials"*, D.-Y. Wang, **Leibniz Institute of Polymer Research Dresden (IPF)**, Leibniz, Germany, October 2017.
31. *"General energy-entropy-momentum integration methods for non-linear themomechanics"*, I. Romero, **Department of Mechanical Engineering, Chemnitz University**, Chemnitz, Germany, October 2017.
32. *"Multiscale simulation of composite materials"*, C. S. Lopes, **University Carlos III**, Madrid, Spain, October 2017.

33. *"Novel approaches in bio-lighting technologies"*, R. D. Costa, **Helmholtz Zentrum München**, München, Germany, October 2017.
34. *"Microstructure based simulations of polycrystalline metals"*, J. Segurado, **Carlos III University**, Madrid, Spain, November 2017.
35. *"The future of the lighting"*, R. D. Costa, **Emtech**, Barcelona, Spain, November 2017.
36. *"Técnicas de simulación para Materiales Compuestos: una perspectiva multiescala"*, C. González. **Webinar of AEMAC (Spanish Association of Composite Materials)**, Madrid, Spain, November 2017.
37. *"Bio-inspired white hybrid light-emitting diodes"*, R. D. Costa, **University of Colorado**, Denver, USA, November 2017.
38. *"New advances in physical simulation of metallurgical processes"*, I. Sabirov. Department of Materials Science and Metallurgical Engineering, **Polytechnic University of Catalonia**, Barcelona, Spain, December 2017.
39. "*A case of success BioLED*", R. D. Costa, **Masquelared**, Castello, Spain, December 2017.

3.8. Awards

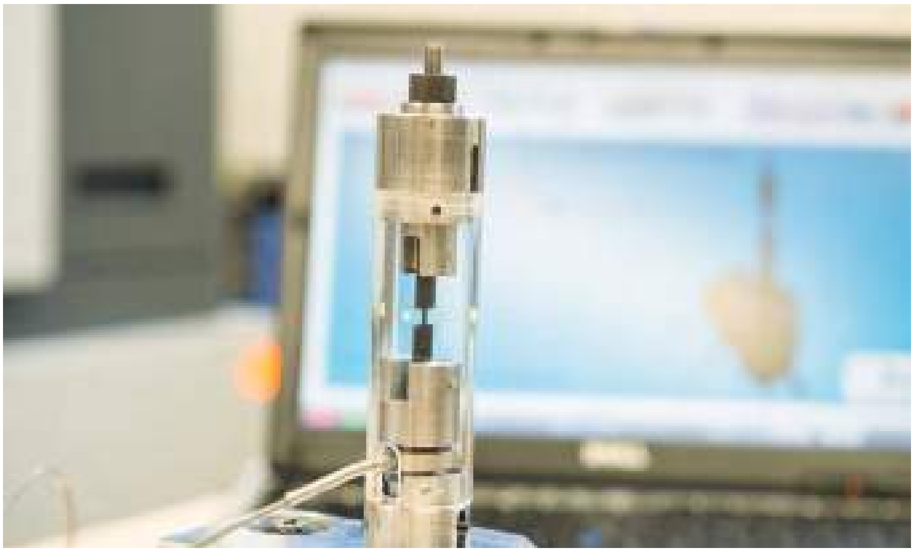
1. 2017 European Innovator (Pioneer) under 35, MIT Technology Review.
   Dr. R. D. Costa.
2. 2017 Spanish Top Talent under 35, MIT Technology Review.
   Dr. R. D. Costa.
3. 2017 ADUC-Jahrespreis 2017, GDCh.
   Dr. R. D. Costa.
4. Elected to the Board of Directors, Society of Engineering Science (SES)
   Prof. J. LLorca
5. Appointed to Chairman of the European Mechanics of Materials Conference Committee (EMMCC)
   Prof. J. LLorca
6. Best poster award, CALPHAD 2017 Conference, Saint-Malo, France, June 2017
   J. Wang

3.9. Seminars

1. *"Solidification of alloys across length and time scales"* **Dr. Damien Tourret** (from Los Alamos National Laboratory). January 2017.
2. *"Structural materials for Gen IV reactors"* **Dr. Marta Serrano** (from CIEMAT, Division of Materials of Energy Interest). January 2017.
3. *"Recent advances and challenges in Li- and post-Li- ion batteries"* **Prof. José Luis Tirado** (from University of Cordoba). January 2017.

4. *"3D printing of medical devices and bioprinting of tissues"* **José Manuel Baena** (from BRECA Healthcare and REGEMAT 3D). January 2017.
5. *"Improving the damage resistance of 6xxx series aluminum alloys by friction stir processing – towards an ERC project"* **Dr. Aude Simar** (from Université Catholique de Louvain). January 2017.
6. *"Incorporating elastoplastic models in phase field"* **Dr. Efim Borukhovich** (from Royal Institute of Technology (KTH) Sweden). February 2017.
7. *"A Manifold learning approach to data-driven computational elasticity and inelasticity"* **Prof. Elias Cueto** (from University of Zaragoza). February 2017.
8. *"Multi-scale mechanistic interpretations to indentation experiments across material length scales: from continuum to atomistics"* **Prof. Jorge Alcalá** (from the Polytechnic University of Cataluña). March 2017.
9. *"Fire protection of films, fabrics and foams achieved through surface nano-structuring"* **Prof. Jenny Alongi** (from University of Milan). April 2017.
10. *"Introduction to machine learning with python: Image processing and recognition"* **Prof. Raúl Sánchez-Martín** (from Ericsson). April 2017.
11. *"A general overview on multiple necking and fragmentation problems in ductile solids subjected to high strain rates"* **Prof. José A. Rodríguez-Martínez** (from the University Carlos III of Madrid). April 2017.
12. *"Innovative materials for nanocrystalline solar cells"* **Dr. Maria Bidikoudi** (from Institute of Nanoscience and Nanotechnology (INN)", Aghia Paraskevi Attikis). May 2017.
13. *"Hybridization and mesotructuring as tools towards functional photocatalysts"* **Prof. Dominik Eder** (from Technical University of Vienna). May 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.
16. *"Glissile junctions: Insights from discrete dislocation dynamics and development of a continuum model"* **Dr. M. A. Stricker** (from Karlsruhe Institute of Technology). July 2017.
17. *"Alloys-by-Design: Optimisation of compositions of Nickel-based superalloys"* **Prof. Roger C. Reed** (from University of Oxford). July 2017.
18. *"Accelerated discovery and development of high temperature structural alloys"* **Dr. Michael Titus** (from Purdue University). July 2017.
19. "Stick–slip dynamics of flow-induced seismicity on rate and state faults"
20. **Prof. Luis Cueto** (from the Technical University of Madrid). July 2017.
21. *"An overview of naturally derived polymers for medical and fibre applications"* **Prof. Maurice Collins** (University of Limerick). July 2017.

22. *“Microstructure informed constitutive models and SPH crystal plasticity modelling approaches”* **Dr. Anxin Ma** (from IMDEA Materials Institute). September 2017.
23. *“Low-dimensional nano-carbons: Form doped carbon nanotubes and doped graphene to 3-D Hybrids and biological applications*” **Prof. Mauricio Terrones** (from Penn State University / IMDEA Materials Institute). October 2017.
24. *“Microbial electrochemical technologies and waste water treatment: Concepts and main applications”* **Dr. Juan Manuel Ortiz** (from IMDEA Water Institute). October 2017.
25. *“Rational design of conducting redox polymers for electrical energy storage*” **Prof. Martin Sjödin** (from Uppsala University). October 2017.
26. *“Design, fabrication and commercialization of new catalysts engineered at the nanoscale”* **Prof. Javier García Martínez** (from the University of Alicante). November 2017.
27. *“The PRISMS framework: An integrated predictive multi-scale ICME capability for the global materials community”* **Prof. John Allison** (from University of Michigan). December 2017.
28. *“An experimentally-accessible library of ordered microporous carbon schwarzites via zeolite-templating*” **Prof. Efrem Braun** (from UC Berkeley). December 2017.
29. *“Decentralized Chemical Sensing: From materials to real world applications”* **Prof. Gastón A. Crespo** (from KTH, Royal Institute of Technology). December 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 nicriestructura 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

17. *"Estudio de la influencia de la segregación en el comportamiento mecánico de aleaciones de magnesio"*
Student: Patricia Lopesino
Technical University of Madrid
Advisor: Dr. Teresa Pérez Prado
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. *"Crecimientohidrotérmico 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

19. *Bio-Inspired materials for hybrid optoelectronics*
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

21. *"Thermal-mechanical characterization of bio-composites"*
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_6Al_4V 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 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. *"Mateirals 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 (SEMNI)*
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.*

3. *Participation in the "European Researchers' night 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*