institute imdea materials

excellence
as our technological key

imdea **materials** institute

annual report

2018

www.materials.imdea.org

Ignacio Romero
Director, IMDEA Materials Institute
March 2019

annual report

2018

www.materials.imdea.org

Ever since IMDEA Materials Institute started in 2007, our growth in terms of economic activity, research results, and impact has been steady. In particular, 2018 has been, in many respects, our most successful year to date. To show a few metrics, the amount of funds from projects and fellowships executed has grown by 52%, our JCR publications increased 49%, and the number of cited works grew 25%. Another scientific highlight of the year 2018 is the grant of the third ERC project of the institute, to be carried out in the group of Hybrid Optoelectronic Materials and Devices.

Parallel to this increase in scientific production and activity, the number of research groups has remained almost constant for several years now. These two apparently contradicting facts can be explained by noting that most group leaders were hired at a relatively young age and are now becoming established researchers. A constant effort shared by all management is to provide the best environment possible so that research can flourish with the least resistance. These working conditions, and our increasing scientific recognition, should help to make our centre a desirable destination for pre- and post-doctoral students wishing to start a career in Material Science.

Looking more carefully at the data in the report, one notices that collaborative projects with industry have experienced a phenomenal growth in the last year. Part of this increase can be explained by macroeconomic conditions, but we are certain that the main reason for this success is the outcome of the three *Strategic Research Projects* launched internally two years ago, aimed precisely at reverting a slowing industrial activity. Our growing experience in project execution and the trust we have gained from our industrial partners are also responsible for these results.

A general feeling is that 2018 has been an outstanding year for the Institute. I would like to acknowledge the committed effort of all our researchers, technical staff, and administration. After 10 years of growth, I am aware that the Institute is now reaching a different phase, one of maturity in which our size and activity should reach a stationary state, and we should focus on impact, instead. This is why in 2018 we started working in a strategic plan for the upcoming years, one that should define in which directions we should steer our efforts to honour our mission, transforming society through research in Material Science and Engineering.

words from the director...

annual report 2018

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IMDEA Materials Institute

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about us

The IMDEA Materials Institute, one of the seven Madrid Institutes for Advanced Studies (IMDEA), is a public research centre founded in 2007 by Madrid's regional government. The goal of the Institute is to do research at the forefront of Material Science and Engineering, attracting talent from all around the globe, and collaborating with companies in an effort to transfer fundamental and applied knowledge into valuable technology.

mission

"We do research of excellence in material science, contributing to tackle the challenges of society and fostering the sustainable development of the region of Madrid"

vision

"Our vision for the future is that IMDEA Materials becomes a leading research institute, internationally recognized for its excellence in material science and its contributions to the transformation of society"

The mission and vision of the IMDEA Materials Institute is based in three main pillars:

science

excellence in materials **science** and engineering research

talent

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

transfer

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

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.

- **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**

Societal Challenges

The core strength of the Institute is its international **research team, consisting of talented researchers from 17 different nationalities,** which carries out new scientific discoveries in materials science, and foster the development of emerging technologies.

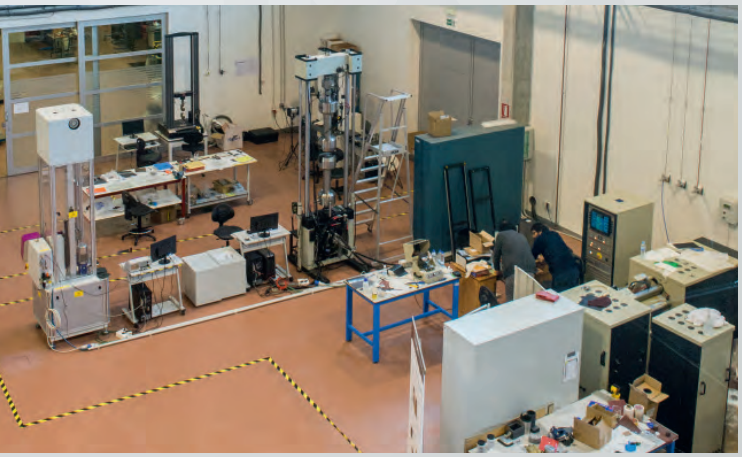
116 researchers

17 nationalities

50% PhDs

48% foreign researchers

16 research groups



The facilities of IMDEA Materials Institute

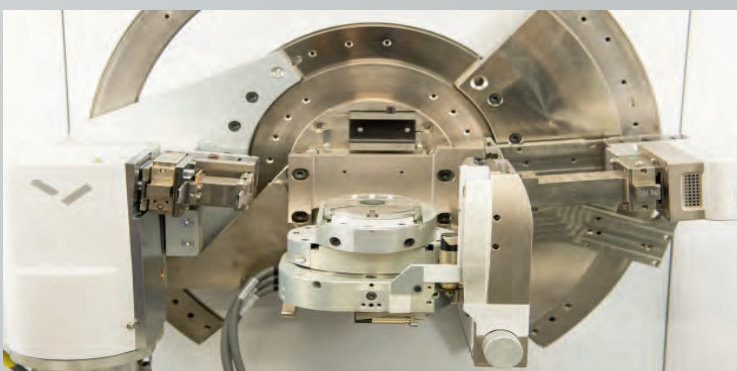
The building and laboratories of IMDEA Materials Institute are located at the Scientific and Technological Park of the Technical University of Madrid in Tecnogetafe, Madrid.

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

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in figures

human resources

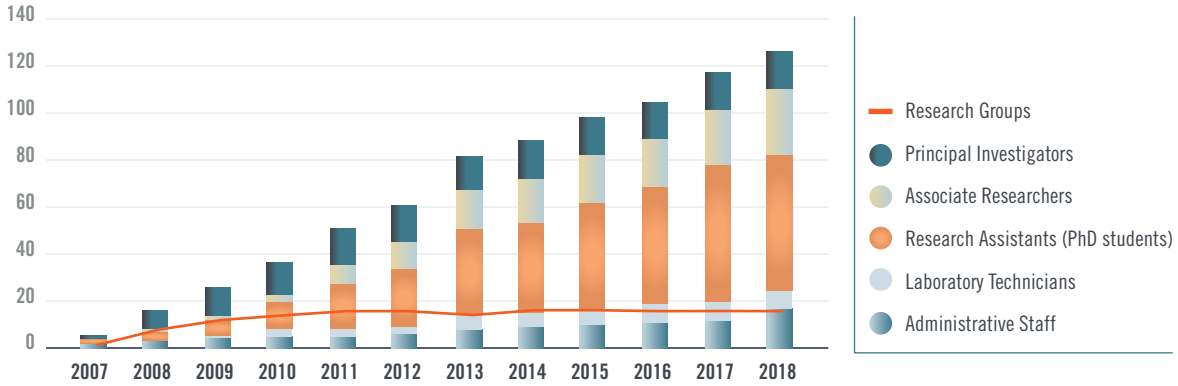
talent

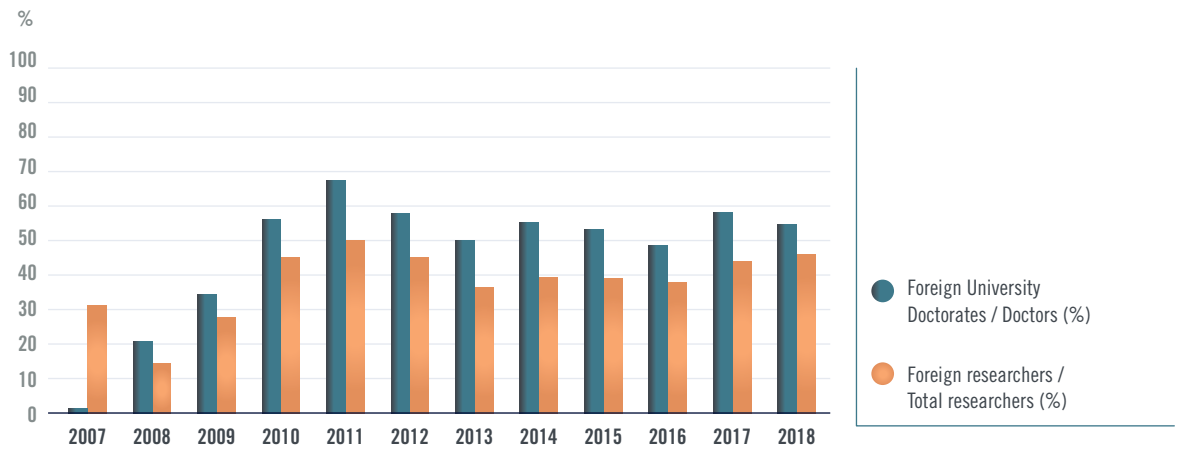
Talent attraction has been the key to the Institute´s **success**.

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**

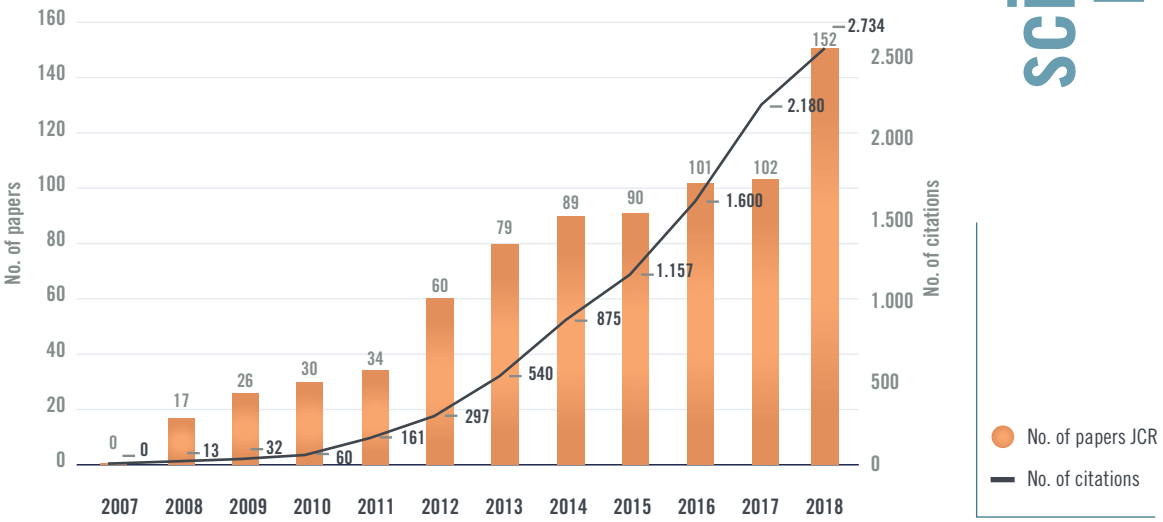
43 defended PhD theses since 2007

60 ongoing PhD theses

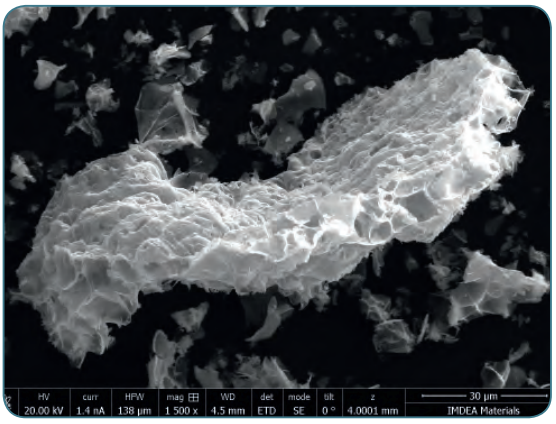
scientific results

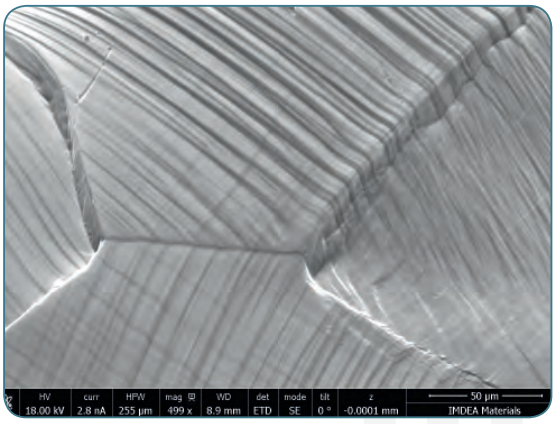
science

The scientific excellence of the Institute is accredited by the evolution of the number of publications (JCR) and citations over the last ten years



2018





56 keynote/ invited talks

152 JCR papers

33 invited seminars

1 patents applied

1 software licensed

2734 number of citations

figures

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 2018

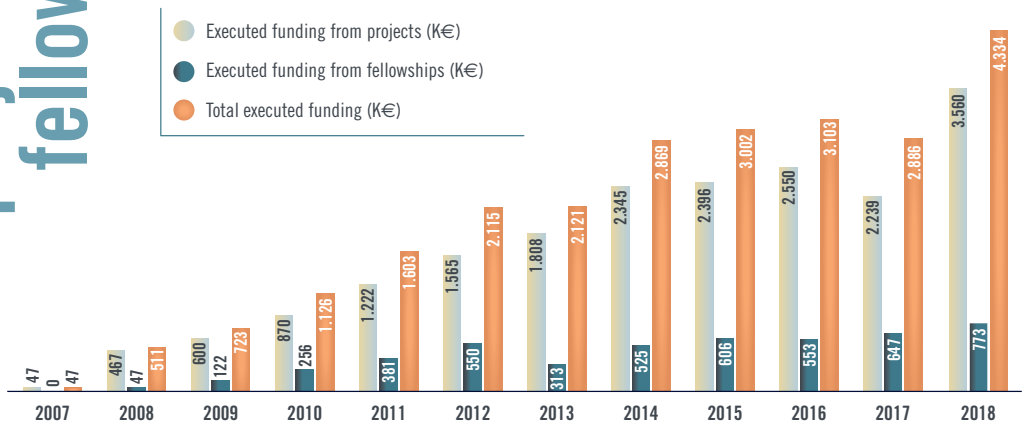
International partnership

IMDEA Materials Institute is the main promoter of the Spain-China joint research centre of advanced materials (JRCAM), established on September 2018.

Members: IMDEA Materials Institute (Co-Director), Beijing University of Chemical Technology, Going Global Confederation of China Petroleum & Chemical Industry, Beihang University, Technical University of Madrid, regional government of Aragón and the companies SANZ CLIMA and REPSOL.

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.



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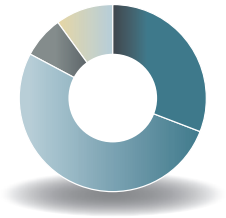


- **International projects** 52%
- **National projects** 7%
- **Regional projects** 10%
- **Contracts with industry** 31%

60
R&D projects

3
ERC projects running

23
R&D contracts with companies

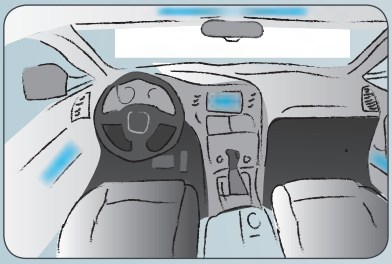
research

talent science transfer

The Institute is currently organised into sixteen **research groups** focused on different areas in the field of materials science and engineering. Each of these groups is led by one staff researcher, who is in charge of coordinating and supervising a research team of post and predoctoral reseachers. The research groups, as key units of the Institute, develop research projects and collaborations to drive the frontier of science of their field forward and transfer knowledge into valuable technology.

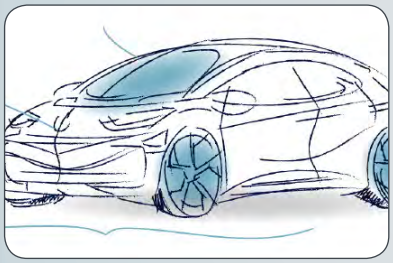
As a result of a high degree of internal collaboration, each research group at the IMDEA Materials Institute participates in several of our **research programmes**. Driven by the talent of the researchers, the research programmes combine cutting-edge fundamental oriented research in topics at the frontiers of knowledge with applied research encompassing the midterm interest of our industrial partners to provide long-term technological leadership.

Advanced Materials for Multifunctional Applications



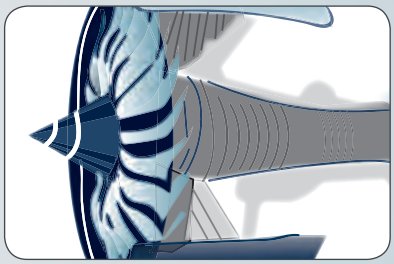
- Synthesis and integration of nanomaterials and polymer-based multifunctional nanocomposites
- New materials and strategies for electrochemical energy storage and conversion
- Hybrid optoelectronic materials and sustainable lighting devices
- Computational and data-driven materials discovery

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...)

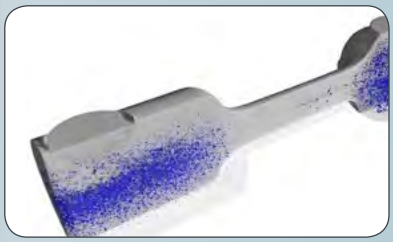
Novel Alloy Design, Processing and Development



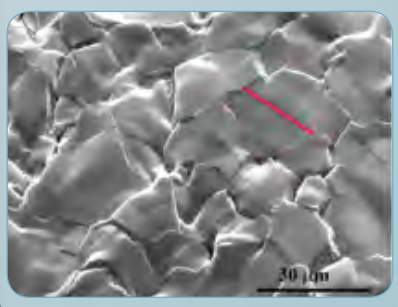
- Structural alloys: light alloys, high temperature alloys and high strength steels
- Characterisation of microstructure and mechanical behaviour
- Advanced Manufacturing: solidification and casting, physical simulation of metallurgical processes (rolling, forging, extrusion...)
- Additive manufacturing: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

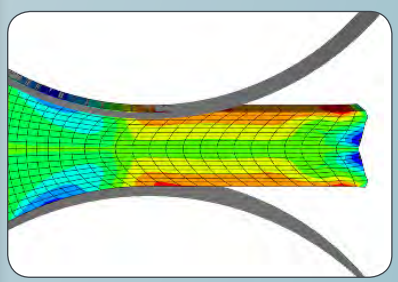


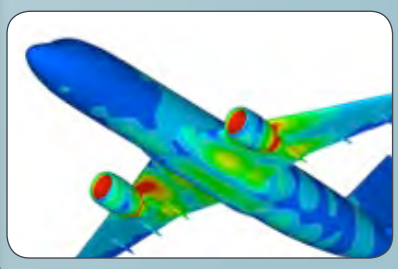
- **4D characterisation:** In-situ characterisation of deformation and processes across multiple length scales (750ºC)



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.

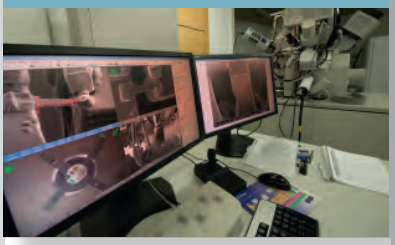
Energy storage and conversion devices

- 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

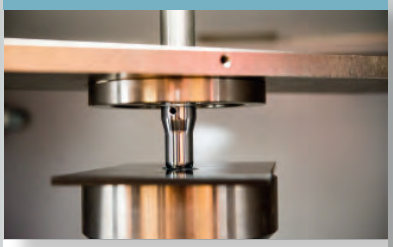
- Fabrication and characterisation of hybrid light-emitting diodes and thin-film lighting devices.
- Rack system consisting of 7 positions that are independently driven, while the luminance and chromaticity features are monitored over time via UV-VIS spectrophotometers coupled to integrated spheres.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

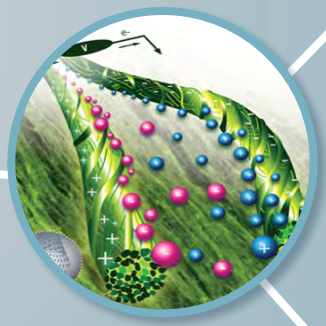
programme
Advanced Materials for Multifunctional Applications

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.

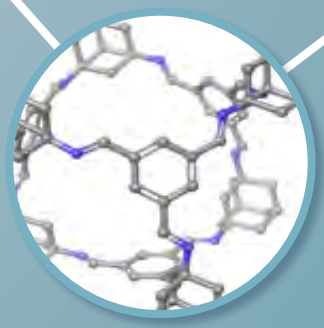
High Performance Polymer Nanocomposites

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

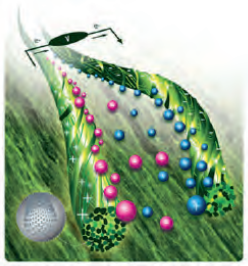
- Design of elastomeric color down-converting materials based on fluorescent proteins.
- Fabrication and analysis of single-point lighting and display systems.
- Further development towards bio-diagnosis and bio-reactor applications.

Electrochemical energy storage

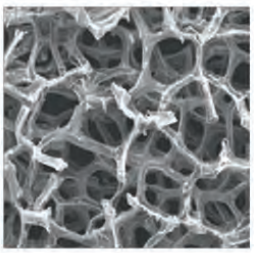
- Tailored designing of nanostructured electrode materials, interfaces and electrolyte compositions.
- Spectroscopic/microscopic studies and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O_2.

Computational and data-driven materials discovery

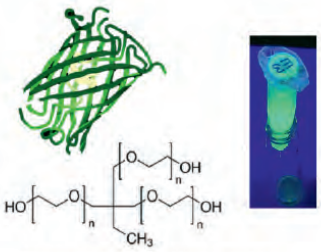
- Discovery of porous materials for energy applications (CO_2 capture, methane storage).
- Design of ionic liquids.
- Characterisation of nanoparticles and others.



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

NAMBAT / Quest for safe and sustainable batteries using Na-ion Mg and hybrid concepts

Funding: 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 2017
Partners: University of Cordoba (Project coordinator) and IMDEA Materials Institute
Project period: 2018 – 2020
Principal Investigators: Dr. Vinodkumar Etacheri and Dr. Maciej Haranczyk

The main objective of this project is to develop advanced Mg-Na hybrid batteries for next-generation electrochemical energy storage. This will be achieved via nanoscale engineering of electrode materials capable of simultaneous Na^{+} and Mg^{2+} storage. Lower molecular weight and doubly charged nature of Mg^{2+} is beneficial in this case for achieving high volumetric energy density. Fire resistant electrolyte compositions and separators will be also developed for improving the safety of the proposed hybrid batteries. Machine learning approach and polymer fabricating techniques are employed for the fire retardant electrolyte formulation and separator fabrication respectively. Na-Mg hybrid batteries developed as part of the proposed project will have high energy/ power density, improved safety and excellent cycle life compared to current generation Mg and Na-ion batteries.

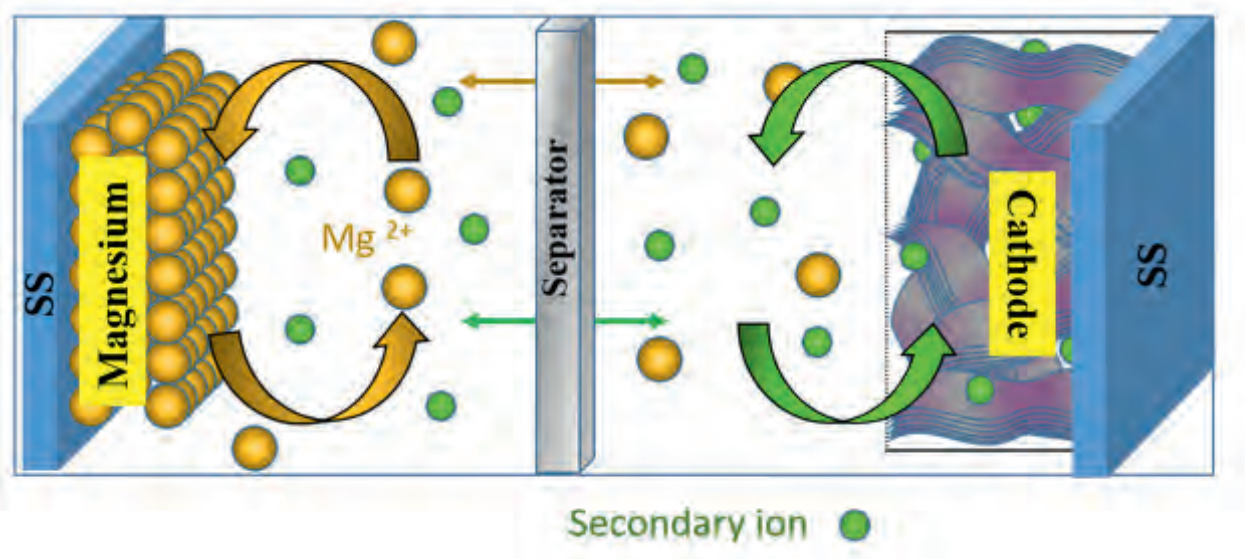


Figure 1. Schematic for Mg hybrid: The magnesium metal perform as the anode where as specially chosen material with specified morphology would perform as the cathode. The charge storage at the anode is dominated by the Mg^{2+} ions however at the cathode the secondary hybrid ion dominates.

ENERYARN / Nanostructured yarn composites for structural energy storage

Funding: European Union, Horizon 2020 Programme (Grant Agreement 797176), Marie Skłodowska-Curie-IF
Project period: 2018 – 2020
Principal Investigator: Dr. Anastasiia Mikhalchan
Supervisor: Dr. Juan José Vilatela

This research is motivated by the ever-increasing need of the aerospace, automotive, and marine industries for novel multifunctional composites with superior structural toughness, capable for energy-storing applications. The proposed topic focuses on the major European societal challenges, such as to reduce weight of transport systems and energy resources consumption, following the European Energy 2020 strategy, Europe 2020 Flagship Initiative, and other climate and energy policies.

The project aims to develop the next generation first-of-this-kind large-scale composites reinforced with carbon nanotube yarns, with improved longitudinal and transverse mechanical properties for further integration as electrodes in structural energy-storing composites. We seek to apply multiscale engineering principles and advanced instrumental analysis to maximize CNT alignment and CNT/polymer nanoscale interfacial properties to produce the high-performance laminates which are not feasible with conventional carbon fibres or discrete nanotubes. Below an example of a carbon nanotube fibre-based battery electrode with improved performance.

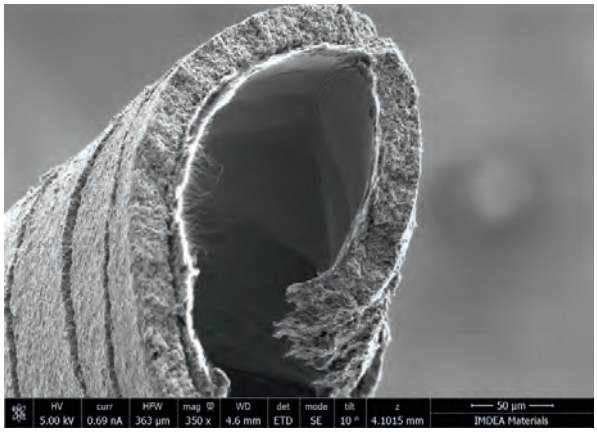


Figure 2. Electron micrograph of a lithium ion battery electrode with carbon nanotube fibre fabric current collector. The composite electrode has 60% higher specific capacity than commercial electrodes, retained even after fracture following tensile deformation above 15%.

Scientific highlights

Cobalt nanoparticles chemically bonded to porous Carbon nanosheets: A stable high-capacity anode for fast-charging Lithium-ion batteries

Cobalt oxide (Co_3O_4), one of the most fascinating magnetic P-type semiconductors is a capable anode material due to its high theoretical capacity (890 mAh/g). Despite of the several advances in the fabrication of transition metal oxide based anodes, obtaining stable cycling performance and good rate performance of Co-based anodes still remains as a great challenge. Herein, we report a facile strategy for substantially improving the Li-ion storage performance of Co-based anodes by chemically bonding Co nanoparticles on porous Carbon nanosheets. Implementation of Co nanoparticles instead of Co_3O_4 restricted Li_2O formation during the charge-discharge process. In-situ formed Co–C bonds during the pyrolysis step improved interfacial charge transfer, and eliminated particle agglomeration. This work highlighted the importance of Co-C bonds for stabilizing the electrochemical performance of Co-based hybrid anodes for rechargeable Li-ion batteries.

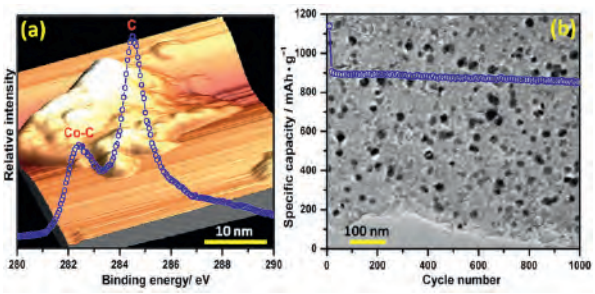


Figure 3. (a) AFM image / C 1s XPS spectra and (b) TEM image/ electrochemical performance of cobalt nanoparticles chemically bonded to porous carbon nanosheets.

Reference: V. Etacheri, C. N. Hong, J. Tang, V. G. Pol, ***ACS Appl. Mater. Interfaces 10,*** 4652–4661, 2018.

White hybrid light-emitting diodes (WHLEDs)

White hybrid light-emitting diodes (WHLEDs) combine a high-energy emitting LED with easy-to-prepare and eco-friendly low-energy emitting organic colour down-converting packings. IMDEA Materials has recently developed one of the most outstanding down-converting materials based on luminescent organometallo-silica nanoparticles. Since 2006, the synthesis methodology has been limited by the incorporation of a single emitter, leading to a moderate color stability in WHLEDs. We have discovered a two-step synthesis protocol based on the kinetic formation of white-emitting organometallic dots with three emitting iridium (III) complexes followed by their transformation into mesoporous silica nanoparticles. WHLEDs prepared with this novel down-converting material feature great stabilities (>2000h) in concert with a sun-like spectrum.

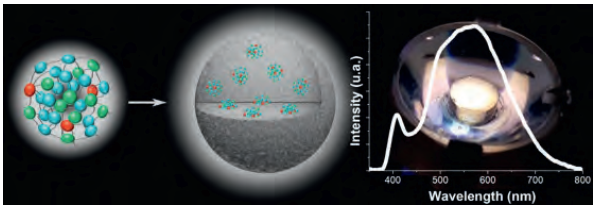


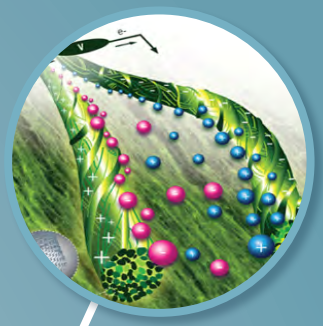
Figure 4. Left. Sketch of white-emitting silica nanoparticles consisting of a core made of blue, green, and red emitters and a silica shell. Right. Picture of a hybrid LED, in which the UV-chip (390 nm) is covered by a color filter with white silica nanoparticles that transform the UV light into sun-like white as shown in the electroluminescence spectrum.

programme
The Next Generation of Composite Materials

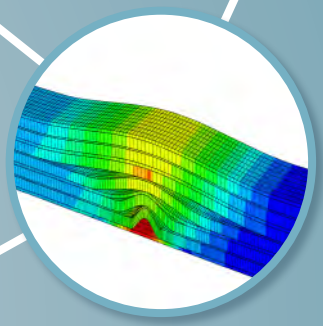
Goal and vision

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.

High Performance Polymer Nanocomposites

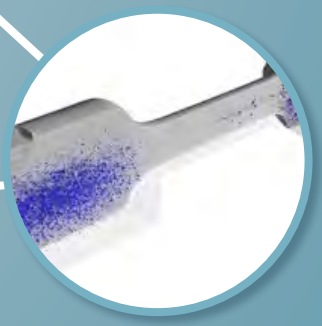


Multifunctional Nanocomposites



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

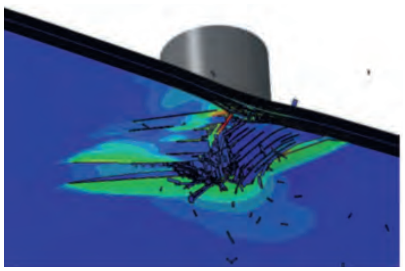
- Multiscale strategies for design and optimisation of composite materials and structures. Behaviour of composite materials and structures under high velocity impact (ice, metallic fragment or blade). Crash-worthiness and failure of composite structures. Effects of defects.

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).



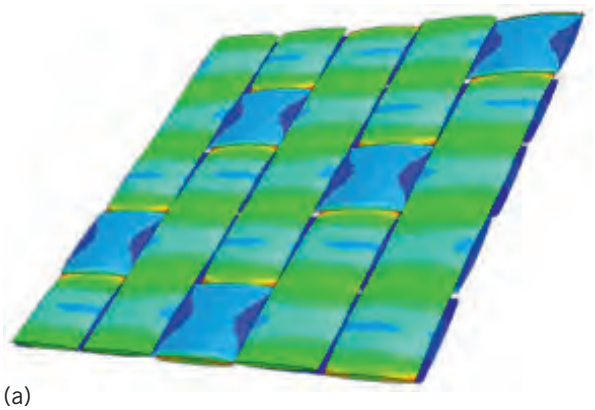
Multiscale virtual testing and processing.

Projects in focus

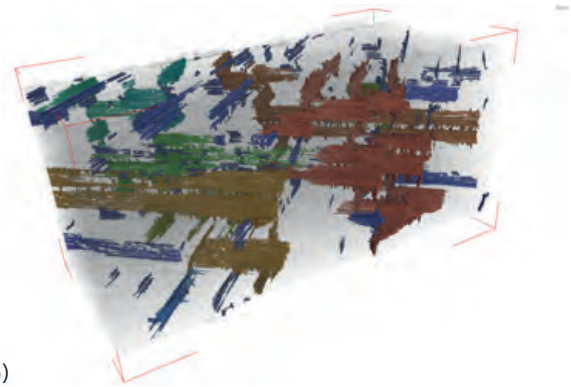
Experimental characterization and numerical analysis of composite materials under thermal and environmental aging

Funding: Regional Government of Madrid. Industrial Doctorate
Partners: Hexcel and IMDEA Materials Institute
Project period: 2018 – 2021
Principal Investigator: Prof. Carlos González

The increased replacement of metals by composite materials in aeronautical structures has presented new challenges to engineers, largely due to the highly complex failure mechanisms of composite materials but also due to the many uncertainties that can exist in the manufacturing of composite components and that may significantly affect the reliability of strength predictions. This is particularly true when dealing with environmental loads as the aircraft undergo continuous temperature and humidity cycles as well the exposure to harsh chemicals and liquids. The combination of temperature and water absorption induces residual stresses during the service life that may produce matrix crack reducing the loading carrying capacity of the material. Understanding the way, the environment affects the structural properties of composites is mandatory to increase their safety and reliability. The project aims to understand matrix cracking progression in different structural composites induced by the environmental aging produced by temperature-humidity cycles as well as harsh chemicals using X-ray computed tomography. This information will help to fully develop multiscale models for composites that allow robust prediction of the mechanical behaviour through the different length scales which will have a tremendous impact in the industry in the following years. The project has been funded through the Industrial Doctorate Program of the Regional Government of Madrid and Hexcel Composites.



(a)



(b)

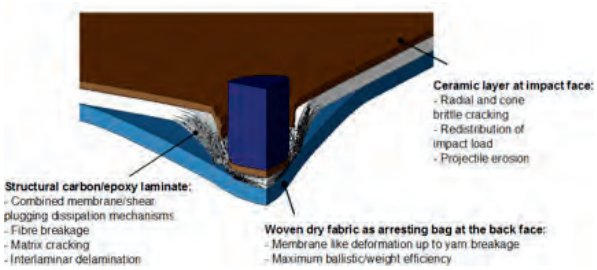
Figure 1. a) Mesomechanical model of a woven textile, b) XCT showing matrix cracking due to thermomechanical loads.

REDISH / CROR engine debris impact shielding. Design, manufacturing, simulation and impact test preparation

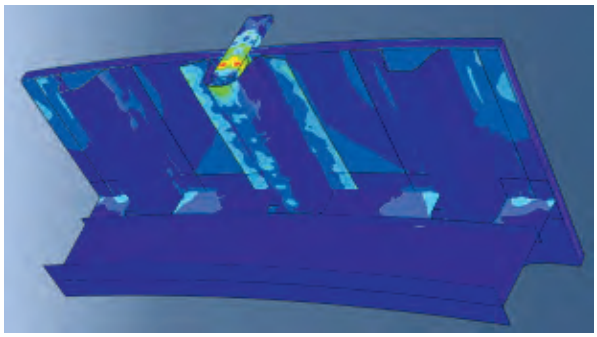
Funding: European Union, Horizon 2020 Programme (Grant Agreement 686946), Clean Sky Joint Undertaking 2
Partners: IMDEA Materials Institute (Project Coordinator) and Foundation for the Research Development and Application of Composite Materials (FIDAMC)
Project period: 2016 – 2019
Principal Investigator: Dr. Claudio Lopes

New, eco-efficient aircrafts are challenged by a demand to significantly reduce the CO_2 and NO_x emissions. To achieve these goals, Airbus is exploring new configurations to integrate advanced engines and propulsion concepts in the aircraft such as the counter rotating open rotor (CROR) engine. Regarding safety, the main issue is the CROR engine debris that can be released with high energy when there is a failure. It is mandatory to develop innovative solutions for panels and shielding able to shield and reduce damage at impact, to secure the airframe integrity, so that aircraft can make safe continuation of flight and landing after engine burst event. The REDISH project is dedicated to the development, maturation and down-selection of an innovative shielding solution able to sustain impacts from CROR engine burst debris while complying with aeronautical structural requirements and standards, namely regarding weight efficiency (the main source for fuel efficiency and reduction of emissions). A coupled experimental-simulation development approach at two structural scales (panel/laminate and component/structural) is being pursued starting from a large pool of possible configurations that are down-selected in successive analysis steps of increasing event fidelity and structural detail until the best solution is reached. Virtual design and testing by means of high-fidelity simulation tools developed by the Composites Materials Group at IMDEA Materials are used to decrease the need for costly physical testing as much as possible and accelerate the shielding development process.

(a)



(b)



(c)

Figure 2. a) Counter Rotating Open Rotor Aircraft Concept, CROR (courtesy of AIRBUS), b) Virtual integration of impact shield configuration on the aircraft structure, c) Virtual design of hybrid multi-material shield against ballistic impact of metallic fragment.

References: D. Garijo, F. Martínez, C.S. Lopes, J. LLorca, C. González, J. López-Puente, J. A. Loya, J. Toral-Vázquez, V. Votsios and E. Martino, Multiscale FE modelling and design of composite laminates under impact, In: C. Zweben and P.W.R. Beaumont (Eds.) Comprehensive Composite Materials II, Vol. 8, Elsevier, 2017.

Scientific highlights

Fibre kinking: From micro to mesomechanics

The strong anisotropy of unidirectional fibre-reinforced composites induces different failure mechanisms depending on the load state. One of the most limiting phenomena is fibre kinking, which is known as the failure mechanism at the microlevel that takes place when the fibres are loaded under longitudinal compression being the failure triggered by the presence of fibre undulations and misalignments. Fibre kinking takes place in most high fibre volume fraction composite materials: as compressive loading increases, fibres rotate and matrix undergoes shear deformation, at some load level the matrix cannot support the shear stress and the system becomes unstable. A simulation of fibre kinking process is presented in Figure 3a) where local unstable rotation of the fibre is clearly evidenced. The research was carried out under collaboration between NASA Langley Research Center (Hampton, Virginia, USA) and IMDEA Materials and the results were published as a NASA Technical Report. Fibre kinking investigation was developed from a multiscale perspective based on both experimental and simulation viewpoints. Micromechanical models were first developed to account for the different failure mechanisms operating at the microlevel including matrix plastic and damage as well as interface debonding and finite deformations. Constituent parameters for fibre, matrix and fibre/matrix interfaces were measured independently using sophisticated experimental techniques, Figure 3b). The micromechanical models were used to homogenize the constitutive response of the composite material into a new continuum-based model of compressive instability in a higher material length scale.

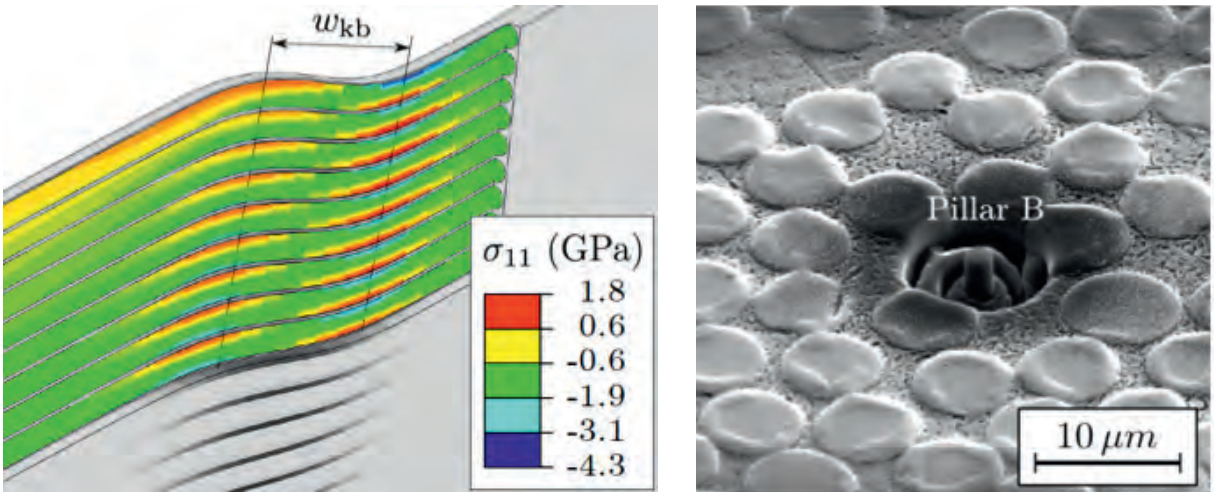


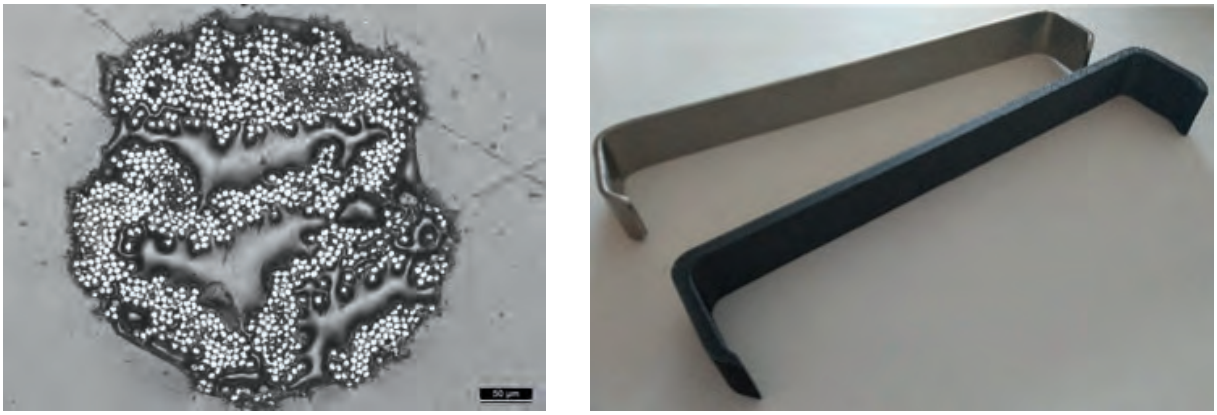
Figure 3. a) FIB milled pillar carved on carbon fibres. Pillars are submitted to compressive load to evaluate the mechanical properties, b) Simulated stress fields in a kink band formed under fibre compressive loads.

Reference: NASA/TP-2018-217743, M. Herráez, A.C. Bergan, C. González, C.S. Lopes, National Aeronautics and Space Administration, Langley Research Center Hampton, Virginia 23681-2199.

Expanding applications of 3D printing of composite applications

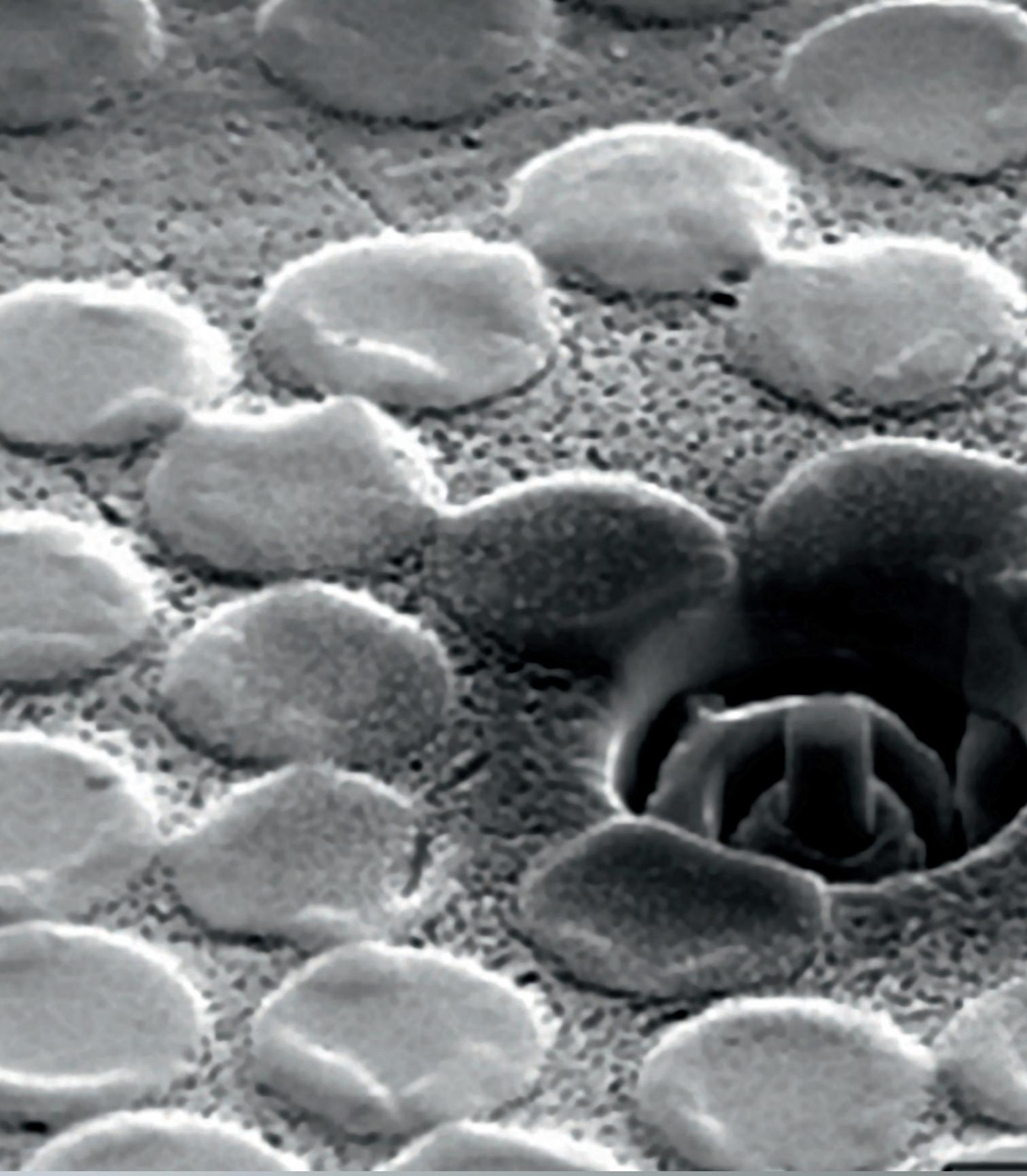
The Next Generation of Composite Materials program is working actively in a research line of additive manufacturing of advance composites materials. The advantages of 3D printing, such as free-design, low cost and rapid fabrication, lead this technology to a great potential for many applications in composite material field in different industrial areas. IMDEA Materials is currently working in this strategic field using one of the 3D printers of long fiber composites available in the market, the MarkForged II. Unidirectional composites made with carbon, glass and Kevlar fibers can be manufactured using the FFF (fused filament fabrication) method. Applications of this technology at IMDEA Materials ranges between production of small-size composite parts for aircraft and automotive industry to the deposition of printed carbon strands on flexible substrates and fabrics acting as advanced sensors for on-off wetting in liquid moulding.

Among the main current limiting drawbacks of 3D printing of unidirectional composites, their low volume fraction of fiber reinforcement, defects and porosities created during fiber track deposition and deficient fiber steering are the most remarkable. The major scientific goal in this area is related to the optimization of raw composite materials and parts optimization produced by FFF, and this task will be carried out by means of a combination of high-level experimental characterisation (micro and meso-mechanics) and the use of advanced multiscale virtual testing tools. Most recently, IMDEA Materials has started to fabricate surgical instruments with specific requirements by tailoring materials, reinforcements and microstructures and, at short-tern, it will develop fiber-reinforced composite materials for 3D printing of bio-implants, with optimized mechanical properties and biodegradability requirements.



(a) (b)

Figure 4. a) Cross-section of a carbon unidirectional filament for 3D printing, b) Carbon 3D printed Farabeuf separator (the metal counterpart is presented in the upper part of the image.



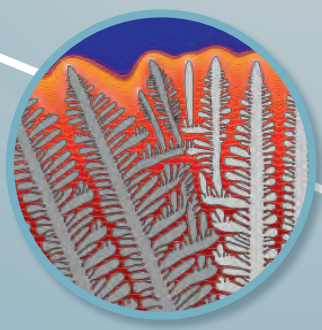
The Next Generation
of Composite Materials

programme
Novel Alloy Design, Processing and Development

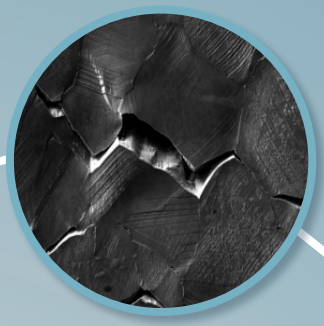
Nanomechanics

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.



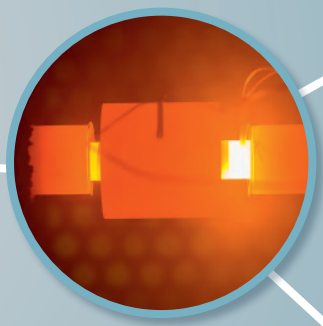
Modelling and Simulation of Materials Processing



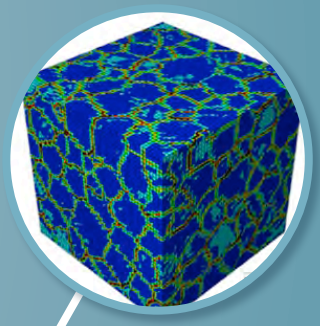
Physical Metallurgy

Solid State Processing

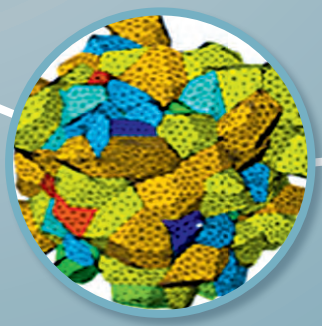
Solidification Processing and Engineering



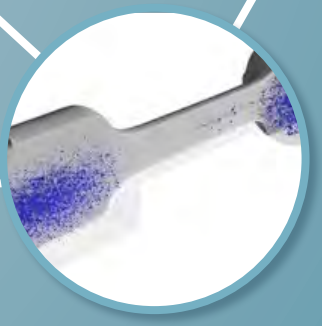
Physical Simulation



Mechanics of Materials



Multiscale Materials Modelling



X-Ray Characterisation of Materials

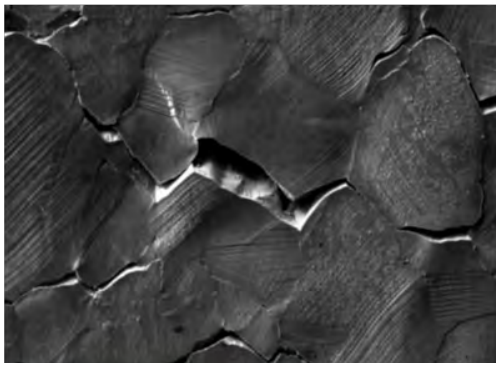
Main research lines

Main research lines

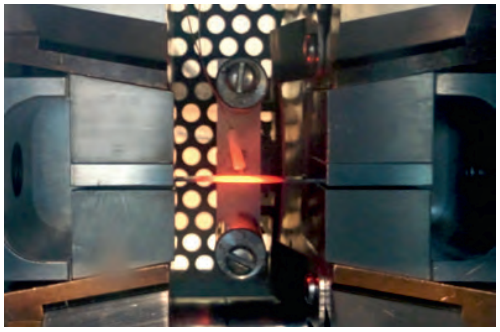
- **Characterisation** of microstructure and mechanical behaviour.
- **Advanced manufacturing:**
  - Solidification and casting.
  - Physical simulation of metallurgical processes (rolling, forging, extrusion, welding).
- **Additive manufacturing:**
  - Powder design and fabrication.
  - Process optimization.
- **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.

Materials of Interest

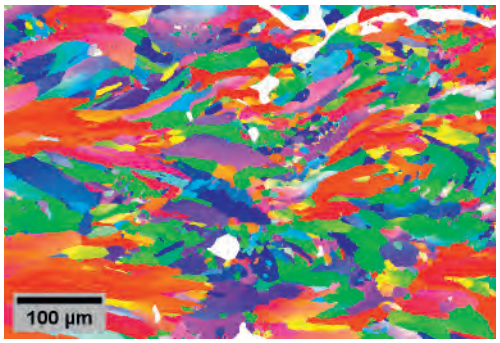
- **Metallic alloys for high temperature structural applications.** Ni/Co-based superalloys, NiAl ,TiAl and FeAl alloys for aeroengine components.
- **Lightweight alloys and their composites.** For biomedical applications (Ti, Mg), electrical applications (Al alloys) or transport (Ti, Mg and nanocomposites).
- **High strength steels.** Quenched and partitioned steels with superior mechanical properties.



In-situ characterisation.



Advanced manufacturing.



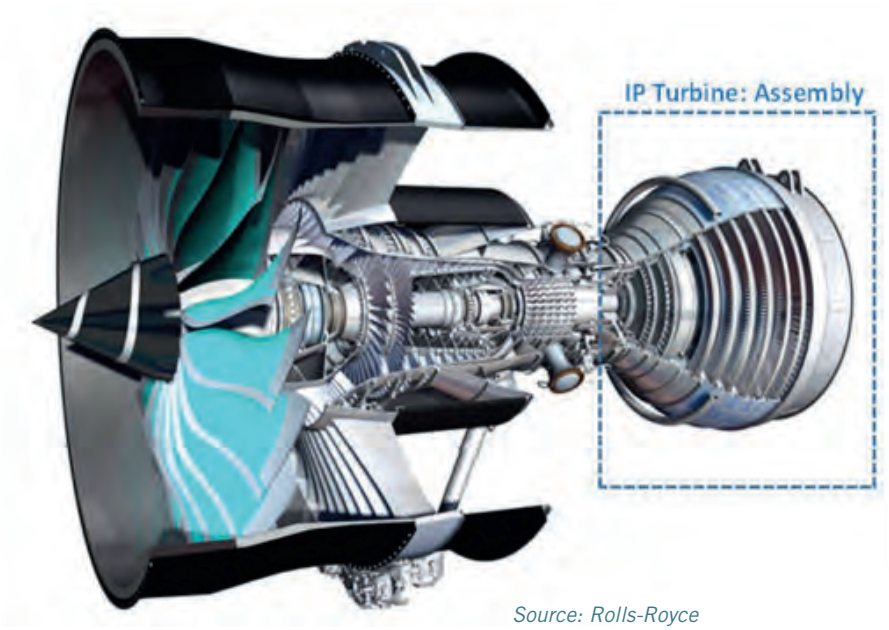
Additive manufacturing (www.industr.com).

Projects in focus

HUC / Development and validation of a powder HIP route for high temperature Astroloy to manufacture Ultrafan® IP Turbine Casings

Funding: Europena Union, Horizon 2020 Programme (Grant Agreement 821044), Clean Sky Joint Undertaking 2
Partners: Centro Tecnológico CEIT-IK4 (Project coordinator), Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali, IMDEA Materiales Institute, Aubert&Duval and Centro de Fabricación Avanzada Aeronáutica – UPV/EHU
Topic Manager: ITP - Aero
Project period: 2018 - 2021
Principal Investigators: Dr. Ilchat Sabirov and Prof. Ignacio Romero

The HUC project focuses on the development of a cost effective manufacturing process based on net shape hot isostatic pressing (NSHIP) of Astrolloy powder to fabricate casings for the Ultrafan® engine. The main objective is to improve the buy to fly ratio of the engine from 9 (achieved through the conventional cast and wrought of IN718) to less than 3 using NSHIP of the material able to withstand engine relevant conditions guaranteeing its ability to contain during service life. The optimized manufacturing route will lead to the optimum powder densification and satisfactory mechanical properties. The research activities cover all the relevant stages of the manufacturing chain, such as powder manufacturing and handling, conditioning, encapsulation, NSHIPing, post-heat treatments and materials characterisation with the ultimate goal for this technology to be fully tested in the relevant UltraFan® demonstrator engine environment. The main contribution of IMDEA Materials lies in the development and validation of modelling tools to predict the containment capability of the developed material during service life.



Source: Rolls-Royce

VITAL / Virtual testing of metallic materials

Luxembourg National Research Fund

Funding: Luxembourg National Research Fund (FNR). Industrial Fellowships
Partners: e-Xstream engineering sarl and IMDEA Materials Institute
Project period: 2018 – 2020
Principal Investigator: Dr. Javier Segurado
Fellow: Dr. Marco Magri

The project ViTaL, "*VIrtual Testing of metallic materiALs*" is a collaborative project between IMDEA Materials Institute and the company e-Xstream engineering sarl with the objective of studying of the deformation and fracture of polycrystalline metals at high temperature. The project is funded by the *Fonds National de la Recherche* (FNR), Luxemburg through the call of *Industrial Fellowship*, and will last from 2018 to 2020. The scientific objectives of the project are developing (1) a continuum coupled model for the deformation by creep accounting for vacancy transport from grain boundaries and (2) a model for fracture of polycrystals relying on a phase-field approach. Both coupled models will be first formulated theoretically and implemented in the multi-field Finite Element (FE) program, *Fenics Project* [1] . In a second stage, the models will be translated to a more efficient framework either FE or using a FFT solver (i.e. FFTMAD [2]). The first results of the model (1) are represented in the Figure 1 where the diffusional creep is simulated in a 2D polycrystal in which grain boundaries act as a source and sink of vacancies as consequence of grain boundary dislocation climb.

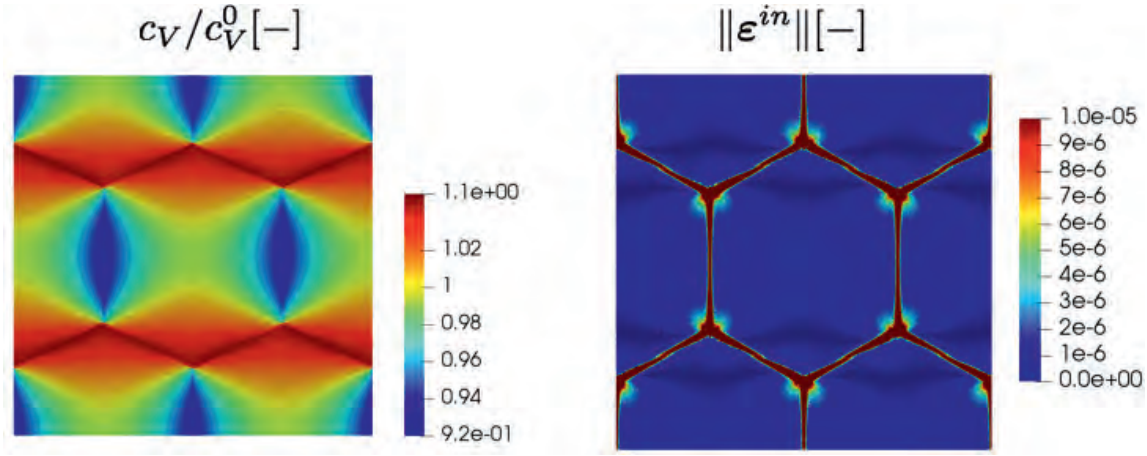
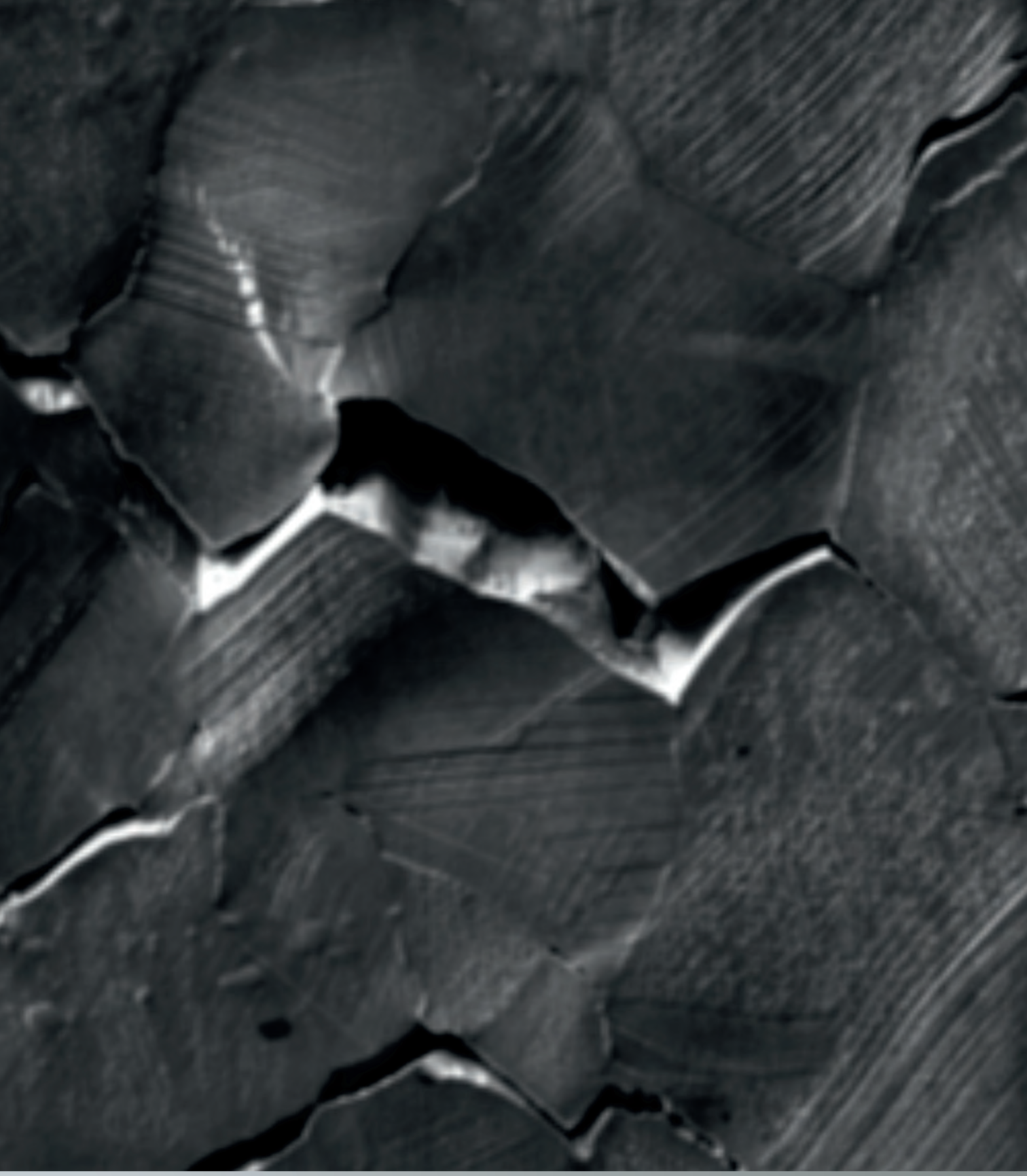


Figure 1. Diffusional creep simulation in a 2D polycrystal (a) vacancy distribution (b) inelastic deformation due to vacancy flux.

This project is one of the activities within the strategic partnership between e-Xstream and IMDEA Materials Institute. This partnership includes the licensing of the crystal plasticity tools developed in IMDEA Materials (CAPSUL) and the scientific consulting work for the development of a new module in the software developed by e-Xstream, DigiMat, for the micromechanical simulation of metallic materials.

References:

[1] M. S. Alnaes, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M. E. Rognes and G. N. Wells, The FEniCS Project Version 1.5, ***Archive of Numerical Software, vol. 3***, 2015.
[2] S. Lucarini and J. Segurado, On the accuracy of spectral solvers for micromechanics based fatigue modeling, ***Computational Mechanics* 63**, 365-382, 2019.



Novel Alloy Design,
Processing and Development

Scientific highlights

Toward more sustainable production of Silicon for solar cells

Photovoltaic energy is considered as a main renewable electric source, and silicon as the dominant material for the fabrication of solar cells. The photovoltaic properties of silicon depend on the concentration of individual impurities, so their levels define the conversion efficiency of solar cells. A demand for solar grade silicon (SGS) is currently surpassing the reserves of the recycled electron grade silicon (EGS), which has been traditionally used by the photovoltaic (PV) industry. Therefore, the metallurgical grade silicon (MGS) is purified by vacuum refining to fill this gap. Besides the elimination of the impurities from metallurgical silicon, it is also important to avoid the contamination of silicon with elements from the furnace during the purification. Graphite is often used for crucibles, substrates, and dyes due to advantages such as high-temperature stability, good machinability and negligible effects of dissolved carbon on the cells efficiency. However, the reactivity between Si and graphite, along with the open porosity are determining factor of the lifetime of graphite crucibles. Therefore, in order reduce the cost of the process and make it more sustainable, new materials for crucibles are needed. Moreover, parameters such as the porosity in crucibles and dies are not controlled at the industry level, so wettability, infiltration, and reaction between silicon and graphite are the key factors in the purification process. Hence, the researchers at IMDEA Materials investigated the wettability, infiltration and reactivity behavior of several substrates against molten silicon by the classic sessile drop method. According to the results, a novel material with superior properties based on carbon fiber composite has been pinpointed. It exhibited higher initial contact angle, better spreading and infiltration behavior as well as less reactivity than graphite. Its use would greatly enhance crucible life, leading to less energy consumption, less Si losses and higher process efficiency, i.e it would make the vacuum refining process of MGS more sustainable.

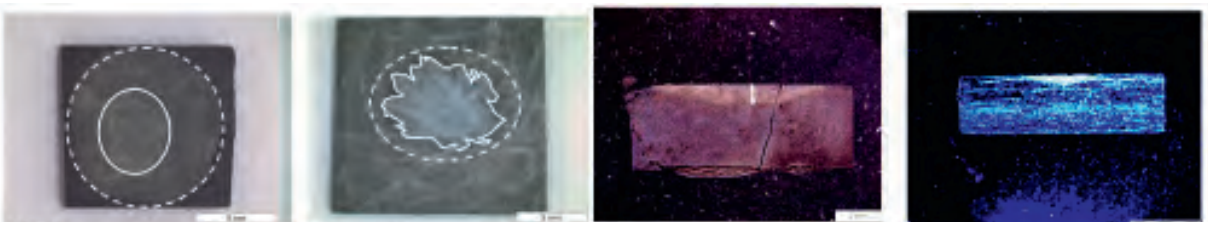


Figure 2. Spreading and infiltration of Si on graphite and composite material.

Digital microstructures from simulations of metallic alloy solidification

Dendrites are ubiquitous in metallic alloy microstructures. They emerge during the growth of solid crystals from the liquid phase during solidification processes, such as casting, welding, or additive manufacturing. These patterns originate from a subtle interplay of mechanisms at distinct length scales – from atomic attachment kinetics at the solid-liquid interface, to macroscopic transport of heat and mass at the process scale. This multi-scale aspect makes dendritic growth particularly challenging to model, such that state-of-the-art phase-field simulations, even massively parallelized on the largest supercomputers, remain confined to a handful of grains.

To address this limitation, IMDEA Materials is developing a multiscale model for dendritic growth. The *dendritic needle network* approach treats dendrites as hierarchical networks of straight branches. By combining physical considerations at different length scales, growth velocities are estimated that fall within a few percent of phase-field predictions. Yet, the numerical discretization can be chosen much coarser, hence accelerating simulations by several orders of magnitude. Making use of a single graphic card for further acceleration, tens of thousands of dendritic branches can thus be simulated on a standard personal computer.

The model has provided accurate predictions of dendritic spacings measured in a range of directionally solidified Al alloys. Thanks to its recent extension to incorporate liquid flow, polycrystalline growth can be simulated under realistic process conditions. Resulting microstructures can now be used in polycrystalline micromechanical models, thus effectively coupling *virtual processing* with *virtual testing*. This is precisely the objective of an upcoming project supported by the European Commission (CINEMA: *Creating an Infrastructure for the Numerical Exploration of Metallurgical Alloys*, MSCA-IF-2018, GA 842795).

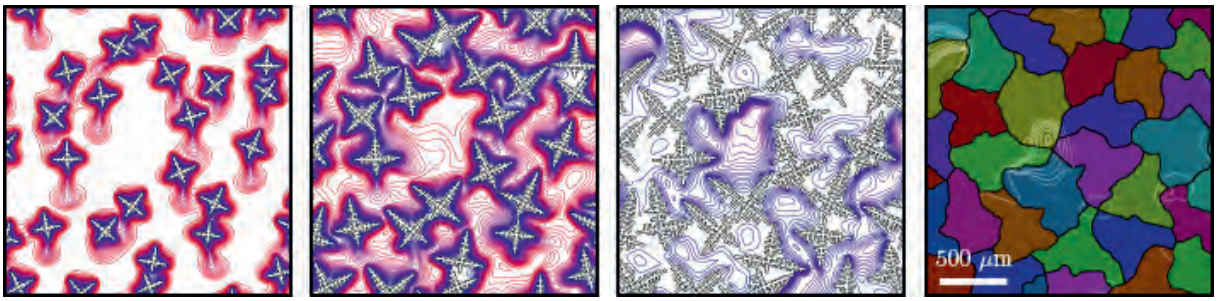


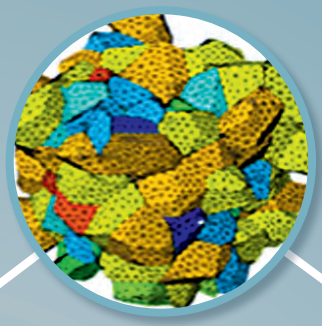
*Figure 3. Multiscale simulation of crystal growth in an Al-10wt%Cu alloy, undercooled by 10°C below its liquidus temperature, in the presence of gravity-driven buoyancy. Time snapshots (left) show the growing crystals (black) and the Cu concentration field (blue-to-red). The final microstructure (right) exhibits irregular grain boundaries (black) and Cu-segregated regions (white). [**Computational Materials Science 162**, 206-227, 2019]*

programme
Integrated Computational Materials Engineering

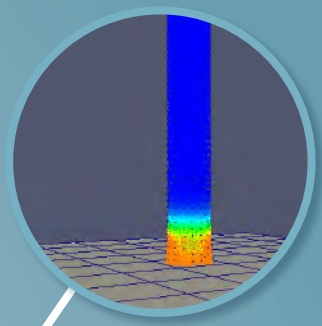
Goal and vision

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.

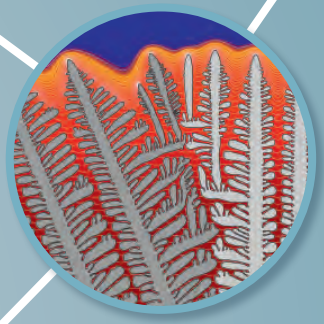
The expertise of the researchers in the programme covers a wide range of simulation techniques at different scales (electronic, atomistic, mesocopic and continuum) and is supported by a high performance computer cluster.



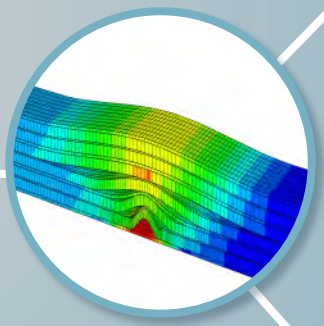
Multiscale Materials Modelling



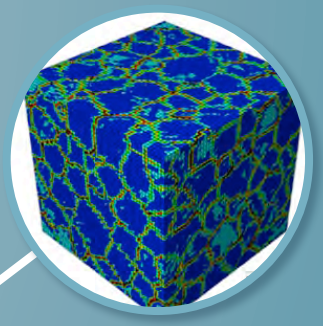
Computational Solid Mechanics



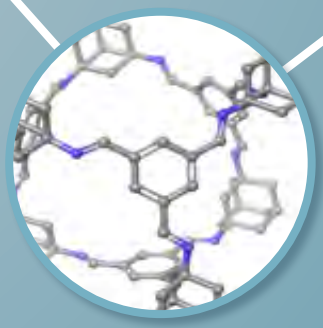
Modelling and Simulation of Materials Processing



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

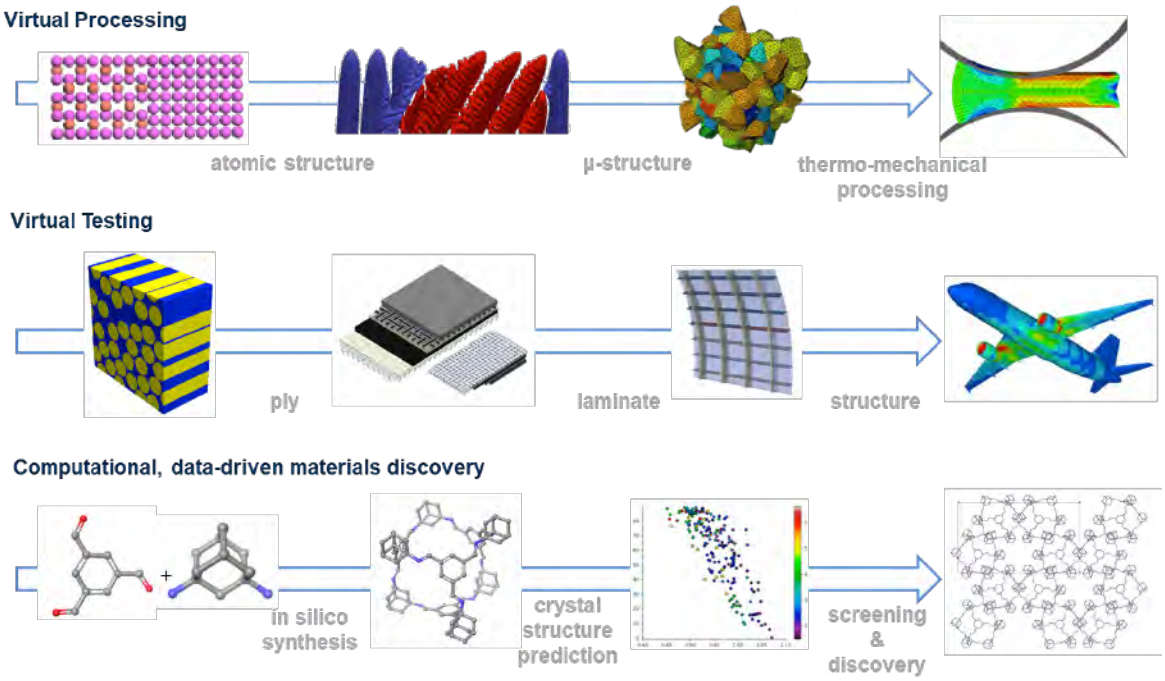
- Light (Al, Mg and Ti) metallic alloys and their composites. Ni-based superalloys. Multifunctional composite materials and structures. Materials for energy generation and storage.

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

ENVIDIA / Virtual environment for the design and manufacturing of airplane turbine engines

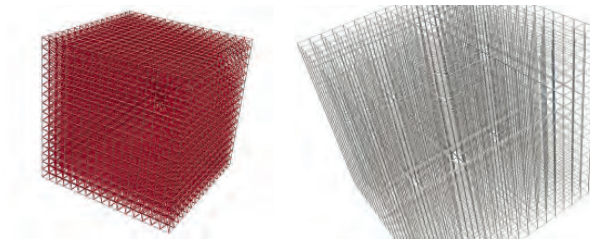
Funding: National Research Agency - Spanish Ministry of Science, Innovation & Universities. National Programme of research, development and innovation oriented challenges of the society. Collaboration Challenges 2017
Partners: ITP Aero (Project Coordinator), Technical University of Madrid, University of the Basque Country and IMDEA Materials Institute
Project period: 2018 – 2020
Principal Investigator: Dr. Damien Tourret

The ENVIDIA project aims at developing simulation capabilities for the design of the next generation of aircraft turbines. In the project, IMDEA Materials focuses on linking processing, microstructures, and properties of Nickel-based superalloys. First, we are developing mechanical simulations of cast components with complex microstructures, combining crystal plasticity theory, computational homogenization of polycrystals, and micro/nanomechanical testing to identify the behavior of individual crystals. Second, we are developing multi-scale simulations of powder-based additive manufacturing (3D printing), combining finite elements, phase-field, and CalPhaD approaches. The outcome of the project will not only accelerate the deployment of future aircraft turbines, but also open the way to the design of novel alloys and the optimization of processes to manufacture metallic components with unprecedented performance and durability in high-temperature applications.

SYMMETRY / Shape memory metamaterials for energy absorption

Funding: National Research Agency - Spanish Ministry of Science, Innovation & Universities. National programme for knowledge generation and scientific and technological strengthening of the R&D&I system. Explore Science 2017
Project period: 2018 – 2020
Principal Investigator: Prof. Ignacio Romero

Artificially engineered lattice structures, also known as metamaterials, are progressively moving from the theoretical realm to practical applications, due to the possibility of 3D printing them. Largely developed for electromagnetic devices, new ideas are emerging for mechanical uses, mostly related to linear wave propagation phenomena. It is widely recognised, however, that a great potential lies on the design of metamaterials whose nonlinear response is harnessed.



In view of these circumstances, the project investigates lattice designs that result in metamaterials capable of absorbing mechanical energy in their nonlinear regime, while having the ability to recover their original shape upon heating. The innovative idea behind these materials consists in realising that elastic structural lattices can be designed whose mechanical response replicates the micro-mechanisms that give rise to the shape memory effect in conventional materials. The project studies the key geometric and energetic requirements for the meso-structure and tests, computationally, new designs

Scientific highlights

FFTMAD - Fast Fourier Transform simulation tool

FFTMAD is a software tool for computational homogenization based on the Fast Fourier Transform algorithm [1,2]. The benefits of FFT based homogenization are the good performance both in CPU time and memory allocation, being much more efficient than Finite Element homogenization

FFTMAD aims to obtain the response of any heterogeneous material, as composites, polycrystals or cellular materials, by simulating the behaviour of a Representative Volume Element of the microstructure. Any macroscopic deformation, stress or mixed history can be applied [2]. FFTMAD includes preprocessing tools for microstructure generation of composites and polycrystals. A set of typical material models are included as elasticity, hyperelasticity, elasto-plasticity and crystal plasticity. In addition, any generic constitutive equation can be used for the behaviour of the materials thanks to a wrapper that allows the direct use of Abaqus-UMAT material-subroutine. FFTMAD solver is parallelised in *GPUs* or *threads* and includes different schemes for linear and non-linear problems. Postprocessing is done using python tools and *Paraview*. FFTMAD is programmed as a Python project and a simulation in FFTMAD is performed by simple scripts defining the RVE, materials, load histories and postprocessing options.

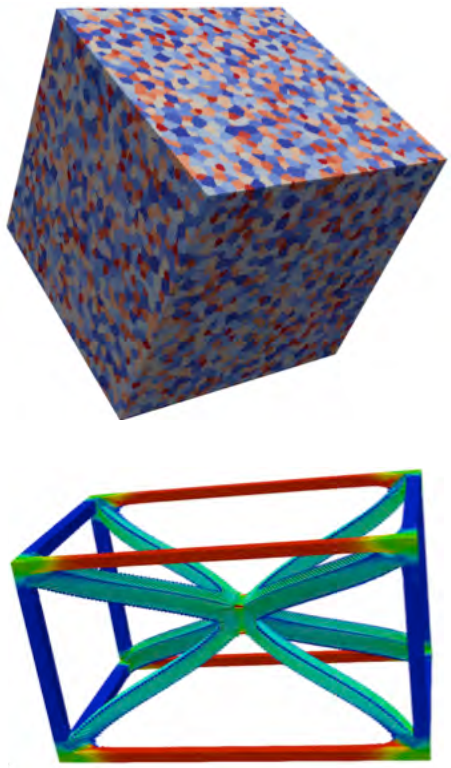


Figure 1. Up: Polycrystaline model containing 120.000 grains and $16{\cdot}10^6$ voxels. Down: Deformation of lattice structure, $2{\cdot}10^6$ voxels

References:
[1] S. Lucarini and J. Segurado, On the accuracy of spectral solvers for micromechanics based fatigue modeling, ***Computational Mechanics* 63**, 365-382, 2019.
[2] S. Lucarini and J. Segurado, An algorithm for stress and mixed control in Galerkin based FFT homogenization. ***International Journal of Numerical Methods in Engineering,*** 2019.

In silico design of porous organic materials

Porous materials are critical to many industrial sectors and are commonly used as membranes, adsorbents for separations, storage and delivery, and heterogeneous catalysts. An improvement of the efficiency of these technologies requires advanced materials that offer unprecedented control over their structure and function. Families of organic and organic-inorganic hybrid extended framework materials and porous cage materials (Figure 1) have been introduced in recent years. Both types of materials benefit from a modular approach to structure design, i.e. their structures, together with their pore chemistry and morphology, can be tuned by selection of building blocks that assemble into functional materials. Our efforts have been focused on the development of computational methodologies to identify molecular/material designs with outstanding properties and performance in various applications. In particular, in 2018 we enumerated and screened a database of 2D and 3D Covalent Organic Frameworks (COF) to identify optimal designs for methane storage application (*Chem. Mater.*, 2018, 30, 5069) as well as demonstrated a prototype of material discovery pipeline for highly porous organic cage materials (*Mol. Syst. Des. Eng.*, 2018, 3, 942).

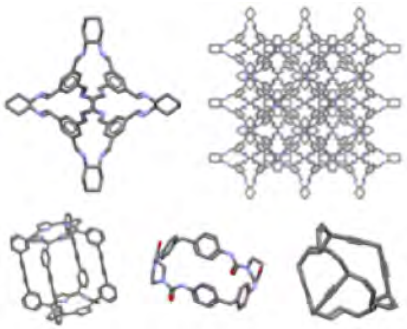


Figure 1. (top row) Example of an imine cage - Covalent Cage 3 and the corresponding crystalline phase; (bottom row) Examples of structural and chemical diversity in cage molecules.

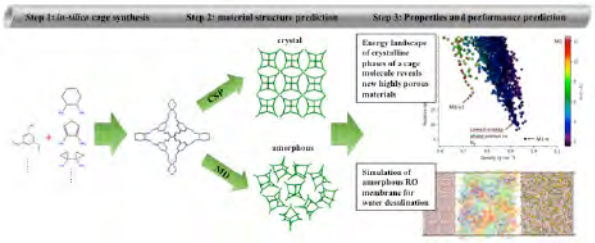


Figure 2. The outline of the developed in silico discovery pipeline implemented for imine cages.

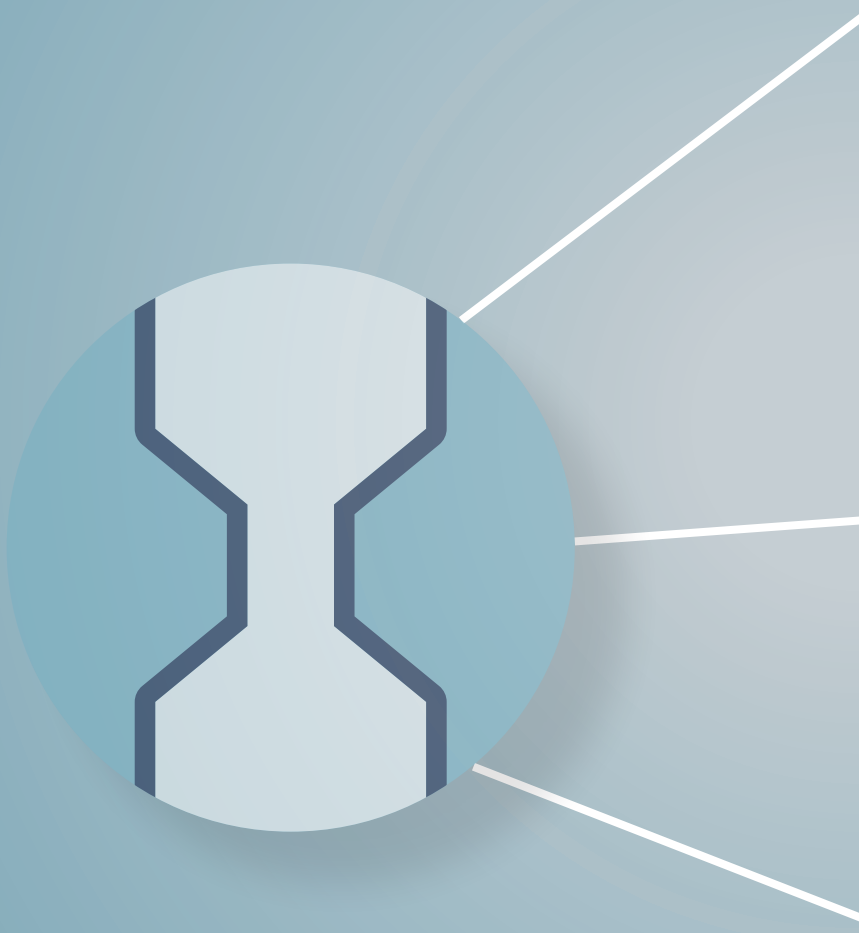
In particular, in regard to the latter porous organic cage materials, our efforts have focused on implementation of the discovery pipeline (Figure 2). Here, we first identify new building blocks by searching large compound databases and combine them to *in silico* synthesize new cages. For each new cage, we perform a crystal structure prediction study followed by the porosity characterization of the predicted phases. Predicted structures featuring interesting porosity properties are further investigated by means of density functional theory calculations and molecular dynamics simulations to assess their thermodynamic stability and performance. Similarly, the cages are also assembled into amorphous solids, which then can be employed as membranes. For example, the performance in reverse osmosis-based water desalination application can be investigated with molecular simulations.

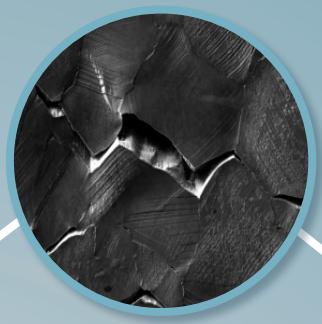
We have demonstrated the prototype of the discovery pipeline in an application focused on a search for highly porous imine cage-based materials. The crystals reported so far based on the imine cages obtained by condensation of 1,3,5-triformylbenzene with several vicinal diamines (1,2-diamine) have rather small pore diameters. For example, the benchmark Covalent Cage 3 (CC3) crystal has a pore limiting diameter of 3.65 Å, and may experience diffusion limitations hindering its technological applications. By applying our screening approach of various CC3 analogues to identify cages that can support stable synthetically accessible, low density porous phases that support pore limiting diameters longer than 10 Å.

programme
Multiscale Characterisation of Materials and Processes

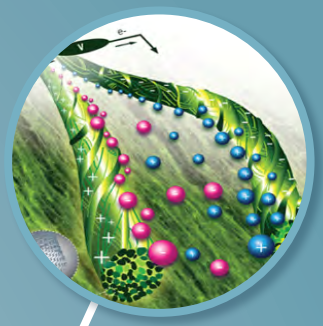
Goal and vision

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.

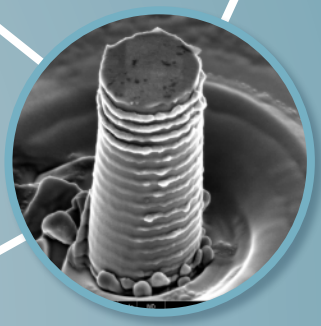




Physical Metallurgy

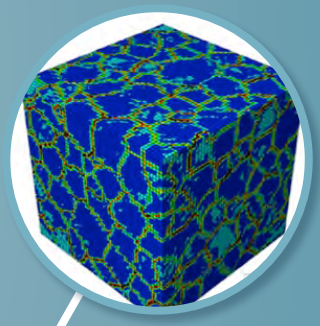


Multifunctional Nanocomposites

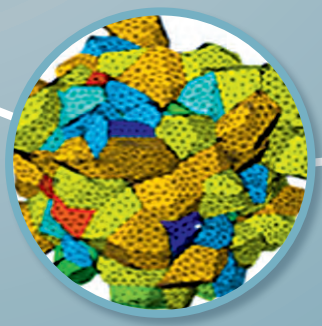


Nanomechanics

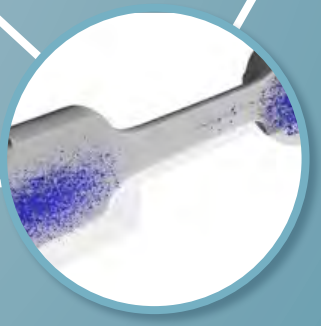
Structural Composites



Mechanics of Materials



Multiscale Materials Modelling



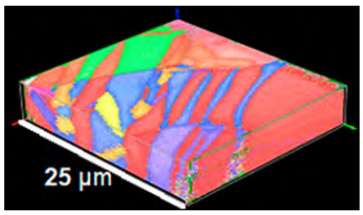
X-Ray Characterisation of Materials

Main research lines

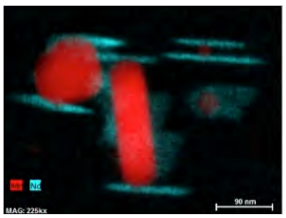
3D characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques:

- 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.

XCT: Porosity in die-cast Mg alloys



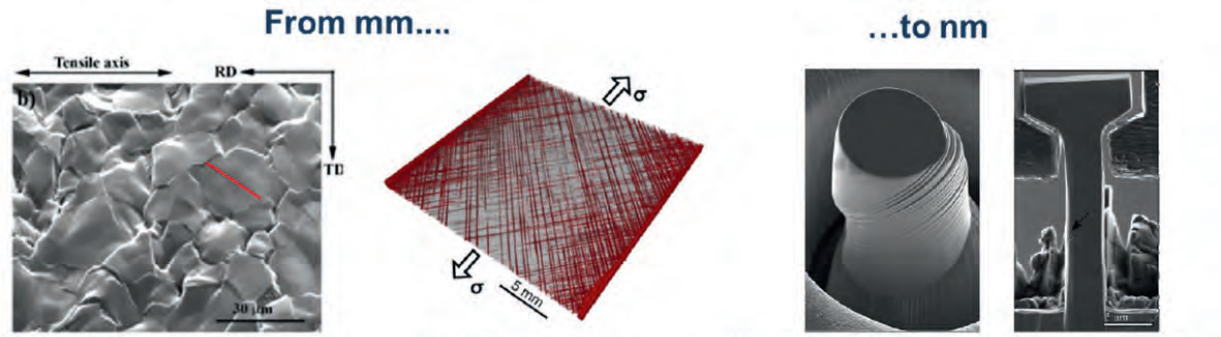
3D-EBSD: Twin structure in a Mg alloy



3D-EDS: precipitates in a Mg-Nd alloy

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.



Deformation of polycrystals in SEM

Composite failure in XCT

Micropillar compression / microtensile testing in SEM/TEM

Cross-correlation between experiments and multiscale simulations (ICME)

Projects in focus

MINIMAL / Characterization of dislocation - Interface interactions in laminates

Funding: European Union, Horizon 2020 Programme (Grant Agreement 749192), Marie Skłodowska-Curie-IF
Project period: 2018 – 2019
Principal Investigator: Dr. Zhilin Liu, Supervisors: Dr. Jon Molina and Prof. J. LLorca

Metallic nanolaminates have attracted great attention due to their superior properties, i.e. large flow strength, high indentation hardness, excellent ductility, good radiation damage resistance, qualified electrical/magnetic response, and promising fatigue/failure resistance. However, better analysis tools are required to design more advanced nanolaminate materials. The objective of MINIMAL is to contribute to the development of these tools by (a) contributing with an in-depth understanding of the physical mechanisms behind dislocation-interface interactions in nanolaminates and (b) developing accurate in-situ mechanical tests at different length scales. Some examples of the progress achieved in this project can be found in the scientific highlights below.

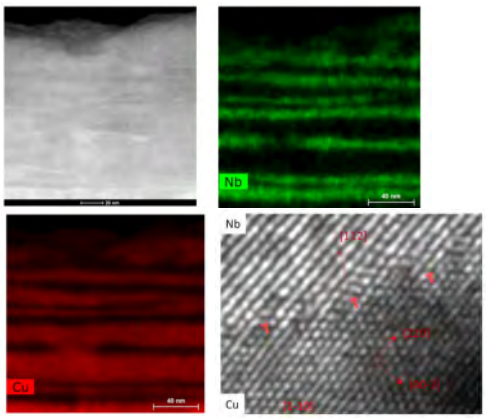
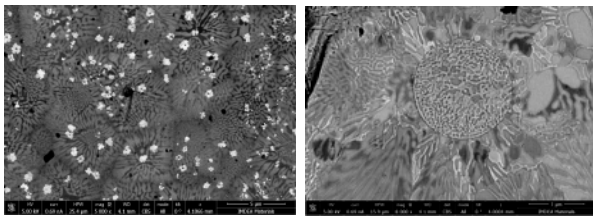


Figure 1. TEM images of a Cu/Nb nanolaminate, showing the Cu and Nb layers and the interface at atomic resolution.

ELAM / Ultrafine eutectics by laser additive manufacturing

Funding: National Research Agency - Spanish Ministry of Economy, Industry and Competitiveness (MEIC) - European Commission/Horizon 2020 Programme – M-ERA.NET 2/ International Joint Actions 2017.
Partners: Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Institut für Werkstoff-Forschung, ACCESS e.V., IMDEA Materials Institute, Fraunhofer Gesellschaft ILT, P&G Manufacturing GmbH, G+L Innotec.
Project period: 2017 – 2020
Principal Investigator: Dr. Federico Sket

The project aims at developing new high strength eutectic alloys by laser-based additive layer manufacturing (ALM) using selective laser melting and laser metal deposition based on Ti-TiFe and Fe-Fe2Ti eutectics. This proposal represents the first attempt to produce ultrafine Ti- and Fe-eutectics by ALM, spanning activities along the entire manufacturing chain from fundamental materials development, powder production, ALM process and post-treatment developments to demonstrator testing.



a) *b)*

Figure 2. Microstructure of the powder alloys atomized for ALM (a) Ti-29Fe-9Sn-5Nb and (b) Fe-15.5Ti in wt%. The eutectic microstructure is revealed by FEG-SEM.

Scientific highlights

Crack propagation in nanolaminates: insights from in-situ TEM tests

In this work, crack propagation as a function of layer orientation was analyzed using in-situ TEM tensile tests (Fig. 1) in Cu/Nb nanolaminates manufactured by accumulated roll bonding. The specimens deformed parallel to the layers presented high ductility and evidence of crack arrest at Cu/Nb interfaces (Fig. 2), while those deformed in the perpendicular direction showed a more brittle behavior, as plastic deformation was rapidly localized in a softer thick Cu layer (Fig. 3). This type of information can only be obtained by in-situ mechanical tests that provide nm scale resolution, as those carried out in the TEM.

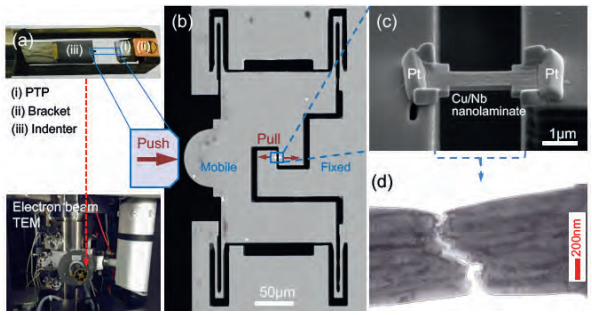


Figure 1. (a) Scheme of the experiment set up (b) Pust-to-pull device to carry out in-situ tensile test in the TEM, (c) Electron transparent specimen, (d) Final fracture of the specimen.

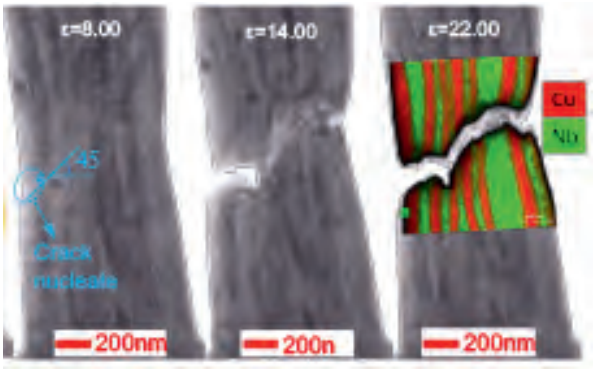


Figure 2. Snapshots taken at different stages of deformation and fracture of a specimen loaded parallel to the layers.

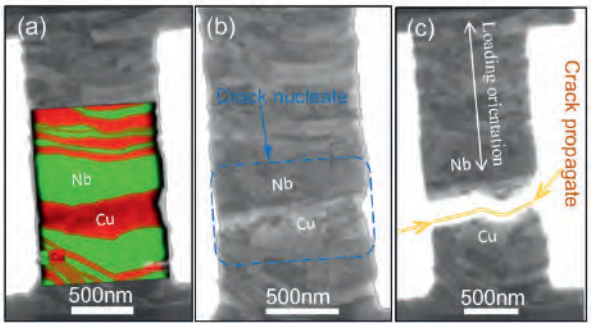


Figure 3. Snapshots taken at different stages of deformation and fracture of a specimen loaded perpendicular to the layers.

Reference: Z. Liu, M. Monclús, L. Yang, M. Castillo, J. Molina-Aldareguia, J. Llorca. ***Extreme Mechanics Letters 25,*** 60-65, 2018.

Understanding the void evacuation process by in-situ curing of OoA prepregs fiber reinforced composites

Void evacuation in OoA composite materials has been a subject of study for many years now. However, till now there was no information on how the voids are evacuated during the curing process. In this work we were able to observe, for the first time, the void evacuation process in 4D, i.e. by carrying out X-ray tomography inspections during the curing process. For that, we have developed an in-situ curing device that allow us to follow not only the void evacuation mechanisms but it also allow us to obtain quantitative information of the resin flow velocity, the efficiency of the so called evacuation path and the effect of the initial microstructure on the final part.

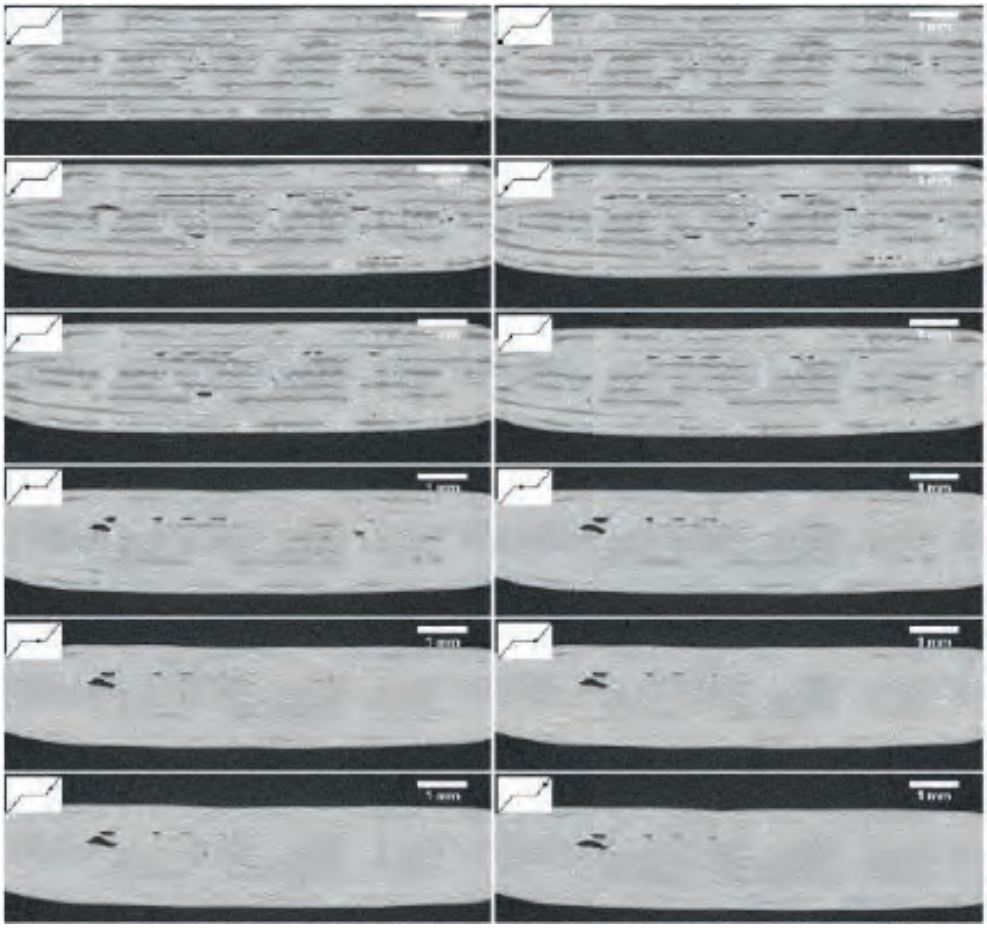


Figure 4. Time sequence as obtained from XCT in the same slice during the curing process of an Out-of-Autoclave composite material. The inset indicates the curing conditions (temperature and time).

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.

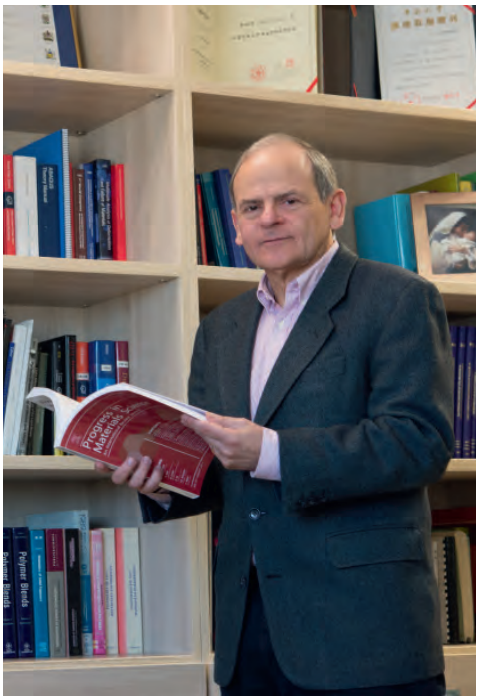
Dr. María Teresa Pérez-Prado

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. WS2, MoS2, NbS2, 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. USA

Professor of Materials Science, Michigan State University. USA

Research Interests

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

Prof. Wen Zhang

Visiting Scientist, High Performance Polymers and Fire Retardants

Ph.D. in Physical Chemistry from Fuzhou University, China

Professor of School of Material Science and Engineering, Fujiang Normal University, China

Research Interests

Porous poly(L-lactic acid) foam; multifunctional monomer modified polypropylene; antibacterial activity of mesoporous zinc oxide; mechanical performance of polymers; rare-earth oxides; organic inorganic hybrid materials.

Dr. Cristian Gebhardt

Visiting Scientist, Solids Computational Mechanics

Ph.D. in Universidad Nacional de Córdoba, Argentina

Research Interests

Computational mechanics and numerical methods; programming and high-performance computing; applied mathematics and differential-geometric methods in mechanics; modelling of mechanical systems, order reduction and optimization; structural dynamics, multibody systems and structure-preserving integration; nonlinear-unsteady low-speed aerodynamics; finite element method and boundary element method; fluid-structure interaction and two-way strong interaction schemes; on- and off-shore large-scale horizontal-axis wind turbines and other forms of wind energy.

Prof. Juan Li

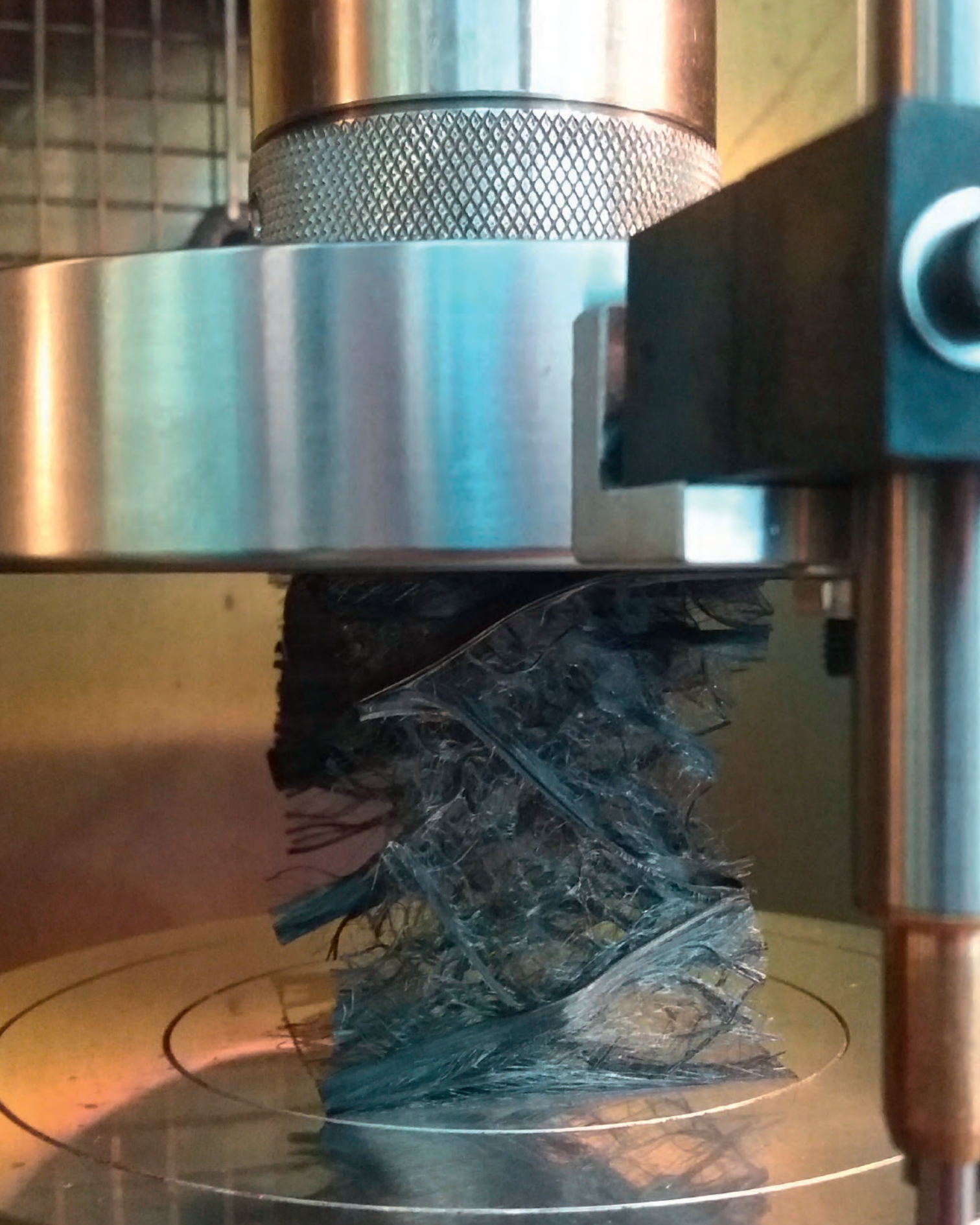
Visiting Scientist, High Performance Polymers and Fire Retardants

Ph.D. in Science, Polymer Chemistry and Physics, Zhejiang University, China

Professor. Polymer and Composites Division, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Science, China

Research Interests

Synthesis of new flame retardant; polymer composites; fire behaviours of polymer-based composites; thermal dynamics of polymer degradation; polymer processing; supermolecule structure; intumescent-like flame retardant; organic-inorganic hybrid material; anti-dripping behaviours; functionalized Carbon nanotubes.



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1. R&D projects and contracts

1.1. European R&D Projects (European Commission)

Title/Acronym: Characterization and Modelling of dislocation interface interactions in metallic laminates at multiple scales /MINIMAL
Partners: IMDEA Materials Institute
Period: 2018 – 2019
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - IF
Principal Investigator: Dr. Zhilin Liu

Title/Acronym: New circular polarized light-emitting electromechanical cells/ NEWPLECS
Partners: IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - IF
Principal Investigator: Dr. Julio Fernández

Title/Acronym: Nanostructured Yarn Composites for Structural Energy Storage/ ENERYARN
Partners: IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - IF
Principal Investigator: Dr. Anastasiia Mikhalchan

Title/Acronym: Development and validation of a powder HIP route for high temperature Astroloy to manufacture Ultrafan IP Turbine Casings/HUC
Partners: CEIT-IK4 (Coordinator), Aubert & Duval SAS, University of País Vasco, Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM), IMDEA Materials Institute
Period: 2018 – 2021
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Clean Sky Joint Undertaking 2
Principal Investigator: Dr. Ilchat Sabirov

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 Commission/Horizon 2020 Programme – Clean Sky Joint Undertaking 2
Principal Investigators: Dr. Srdjan Milenkovic and Dr. Carmen Cepeda

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

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 Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - IF
Principal Investigator: Dr. Xiao-Lin Qi

Title/Acronym: Structural energy harvesting composite materials/STEM
Partners: IMDEA Materials Institute
2016 – 2021
Funding Institution/Programme: European Commission/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 – 2019
Funding Institution/Programme: European Commission/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 Commission/ Research Fund for Coal and Steel (RFCS)
Principal Investigators: 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 Commission/Horizon 2020 Programme – SC5
Principal Investigators: Dr. Srdjan Milenkovic and 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 Commission/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 Commission/Horizon 2020 Programme – COST Actions
Principal Investigator: Dr. Juan Pedro Fernández

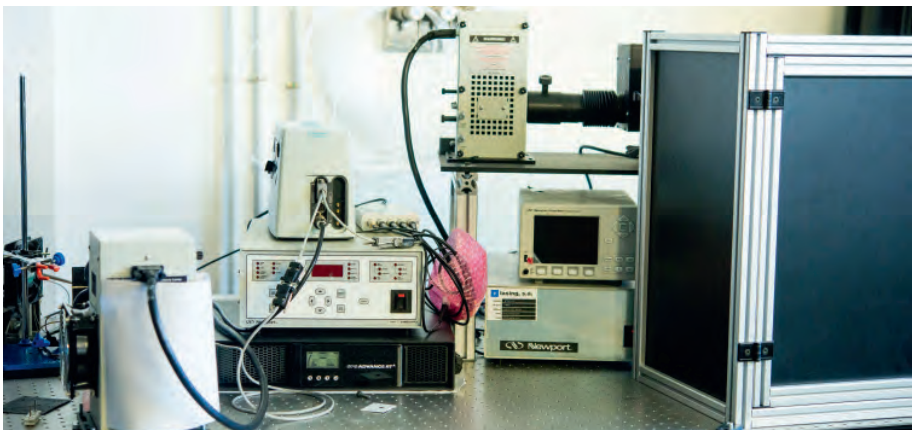
Title/Acronym: Virtual design, processing and testing of advanced metallic alloys for engineering applications/VIRMETAL
Partners: IMDEA Materials Institute
Period: 2015 – 2020
Funding Institution/Programme: European Commission/Horizon 2020 Programme – ERC Advanced Grant
Principal Investigator: Prof.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

1.2. Other International R&D Projects

Title/Acronym: Exploiting low-dimensional properties of carbon nanotubes in macroscopic yarns for charge transfer and storage/NANOYARN
Partners: IMDEA Materials Institute
Period: 2018 – 2021
Funding Institution/Programme: Air Force Office of Scientific Research (AFOSR)
Principal Investigator: Dr. Juan José Vilatela

Title/Acronym: VIrtual testing of metallic materials/VITAL
Partners: e-Xstream, IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: Luxembourg National Research Fund (FNR)
Principal Investigator: Dr. Javier Segurado
Fellow: Dr. Marco Magri

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/Programme: Ministry of Education and Science of the Russian Federation
Principal Investigator: Dr. Ilchat Sabirov



1.3. National R&D Projects

Title/Acronym: Quest for safe and sustainable batteries using Na-ion, Mg and hybrid concepts/ NAMBAT
Partners: University of Cordoba (Coordinator), IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges 2017
Principal Investigators: Dr. Vinodkumar Etacheri and Dr. Maciej Haranczyk

Title/Acronym: Virtual environment for the design and manufacturing of airplane turbine engines/ENVIDIA
Partners: ITP Aero (Coordinator), Technical University of Madrid, University of País Vasco, IMDEA Materials Institute
Period: 2018 – 2020
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 2017
Principal Investigator: Dr. Damien Tourret

Title/Acronym: Shape Memory Metamaterials for Energy Absorption/SyMMEtRy
Partners: IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme for Knowledge Generation and Scientific and Technological Strengthening of the R&D&I system. Explore Science 2017
Principal Investigator: Prof. Ignacio Romero

Title/Acronym: Protein stabilization for luminescent solar concentrators/Pro-CSL
Partners: IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: Fundación BBVA/Becas Leonardo a Investigadores y Creadores Culturales
Principal Investigator: Dr. Rubén Costa

Title/Acronym: Advanced biorubbers for biohybrid lighting and photovoltaic technologies/ INOUTBIOLIGHT
Partners: IMDEA Materials Institute
Period: 2018 – 2019
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy and Competitiveness (MINECO) / National Programme for Knowledge Generation and Scientific and Technological Strengthening of the R&D&I system. Europe Excellence 2018
Principal Investigator: Dr. Rubén Costa

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 Commission/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

1.4. Regional R&D Projects (8)

Title/Acronym: Experimental characterization and numerical analysis of composite materials under thermal and environmental aging
Partners: Hexcel and IMDEA Materials Institute
Period: 2018 – 2021
Funding Institution/Programme: Regional Government of Madrid/Industrial Doctorate
Principal Investigator: Prof. Carlos González

Title/Acronym: Mg alloy, twin band, slip band, fatigue crack, multiscale modelling, insitu Experiment
Period: 2018 – 2022
Funding Institution/Programme: Regional Government of Madrid/Grant for research talent atraction. Modality 1
Principal Investigator: Dr. Anxin Ma

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

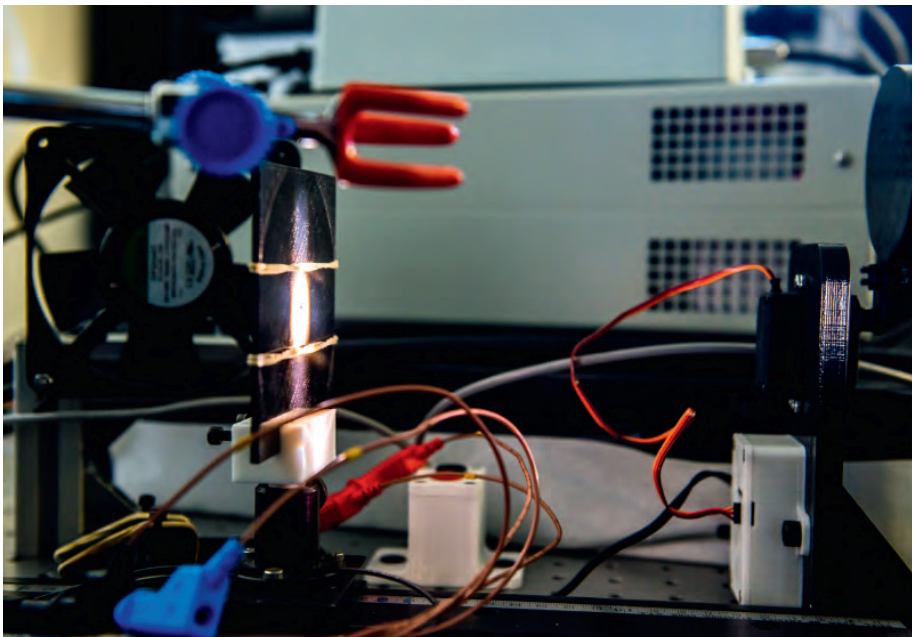
Title/Acronym: The next generation of rechargeable Li-O2 batteries
Partners: IMDEA Materials Institute
Period: 2017 – 2021
Funding Institution/Programme: Regional Government of Madrid/Grant for research talent atraction. Modality 1
Principal Investigator: Dr. Vinodkumar Etacheri

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: Regional Government of Madrid/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: Regional Government of Madrid/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: Regional Government of Madrid/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: Regional Government of Madrid/Programme of R&D activities between research groups in Technology
Principal Investigator: Dr. Juan José Vilatela



1.5. Privately-funded R&D Projects (23)

Title/Acronym: Development of a new transitional element /CONSYS
Company: ANSYS
Period: 2018 – 2019
Principal Investigator: Prof. Ignacio Romero

Title/Acronym: Superalloys for additive manufacturing/SAM
Company: RENISHAW IBÉRICA
Period: 2018-2020
Principal Investigators: Dr. Teresa Perez-Prado and Prof. Javier LLorca

Title/Acronym: Development of advanced materials for lighting applications/POPSICLE
Company: REPSOL
Period: 2018-2019
Principal Investigator: Dr. Rubén Costa

Title/Acronym: Mechanical strength of expanded junctions/UNIEXTEST
Company: ENUSA
Period: 2018-2020
Principal Investigators: Dr. Carmen Cepeda and Dr. Teresa Perez-Prado

Title/Acronym: Preliminary analysis of TiAl containment /PRECONTIAL
Company: ITP Aero
Period: 2018
Principal Investigator: Prof. Ignacio Romero

Title/Acronym: Development of batteries on flexible plastic substrates/BATFLEX
Company: Grupo Antolin
Scientific Partner: IMDEA Energy
Period: 2018 - 2020
Principal Investigator: Dr. Juan José Vilatela and Dr. Rebeca Marcilla

Title/Acronym: Development of a novel flame retardant system for pressure-sensitive adhesive
Company: TESA
Period: 2018-2020
Principal Investigator: Dr. De-Yi Wang

Title/Acronym: Multiscale modelling of the mechanical behaviour of PU foams/ MULTIFOAM
Company: BASF
Period: 2018-2019
Principal Investigator: Prof. Javier LLorca

Title/Acronym: Comparative study of flame retardants for application in polyurethane foams/REPFIRE
Company: REPSOL
Period: 2018-2019
Principal Investigator: Dr. De-Yi Wang

Title/Acronym: High temperature miniature mechanical testing rig for synchrotron tomography/ MACHSYNCH
Company: DLR
Period: 2018-2019
Principal Investigator: Dr. Federico Sket

Title/Acronym: Functionalization of natural brucite and its application in polymers/ TOBEST
Company: Liaoning JINGHUA NEW MATERIALS INC
Period: 2018-2019
Principal Investigator: Dr. De-Yi Wang

Title/Acronym: Alloy design for additive manufacturing
Company: Metal sector
Period: 2018
Principal Investigator: Dr. Damien Tourret

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 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
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: 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

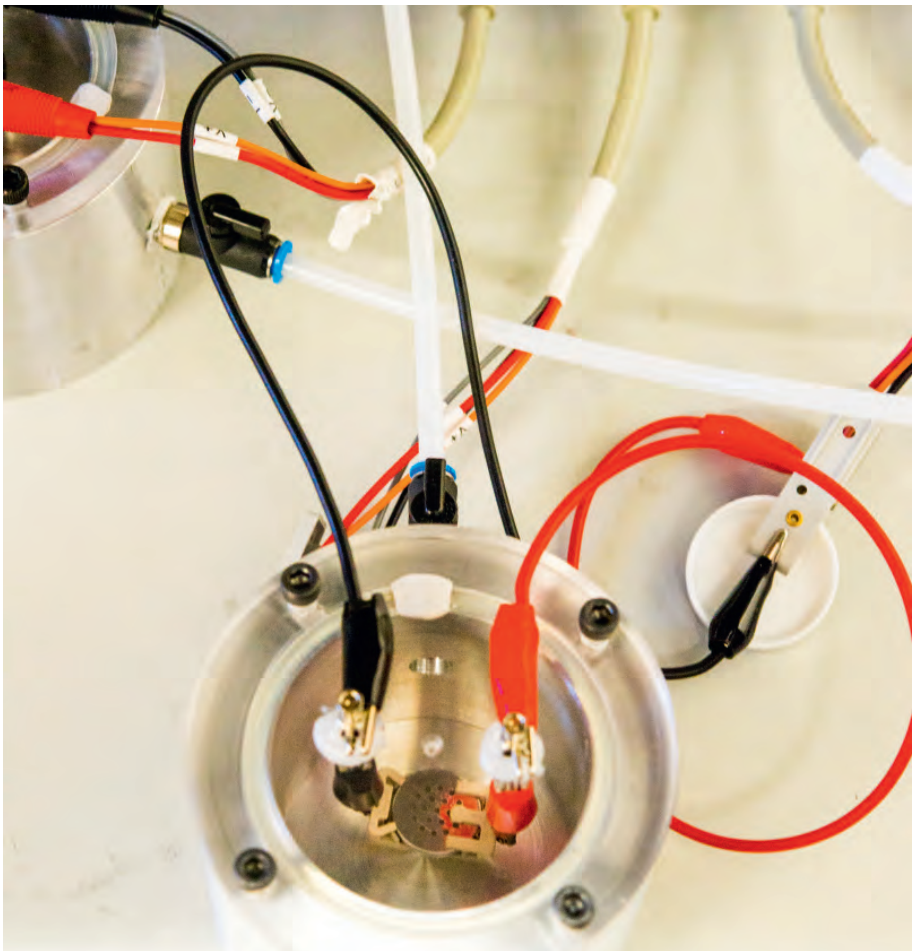
Title/Acronym: Multiscale virtual testing of CFRP samples/VIRTEST
Company: Fokker Aerostructures B.V.
Period: 2014 – 2018
Principal Investigator: Dr. Cláudio S. Lopes

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

1.6. Licenses

CAPSUL - Crystal plasticity software
Licensors: IMDEA Materiales Institute and Technical University of Madrid
Licensee: MSC Software Belgium
Period: 2018 – 2023
Principal Investigator: Dr. Javier Segurado



2. Fellowships

2.1. International

Programme: China Scholarship Council fellowships
Project: New approaches towards perovskite light-emitting diodes
Period: 2018-2022
Funding Institution: China Scholarship Council
Y. Duan

Programme: China Scholarship Council fellowships
Project: Multifunctional CNT fibre supercapacitors
Period: 2018-2019
Funding Institution: China Scholarship Council
C. Meng

Programme: China Scholarship Council fellowships
Project: Relationship between microstructural and mechanical properties and strengthening toughening mechanisms in metastable beta Ti alloys
Period: 2018-2020
Funding Institution: China Scholarship Council
C. Chen

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
Q. Wang

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
P. Xia

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: 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: Juan de la Cierva - Training
Period: 2018-2019
Funding Institution: Spanish Ministry of Economy, Industry and Competitiveness
Dr. R. Alizadeh

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: 2018-2022
Funding Institution: Spanish Ministry of Education, Culture and Sport
A. Rodríguez

Programme: Training University Lecturers (FPU)
Period: 2018-2021
Funding Institution: Spanish Ministry of Education, Culture and Sport
R. Santos

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

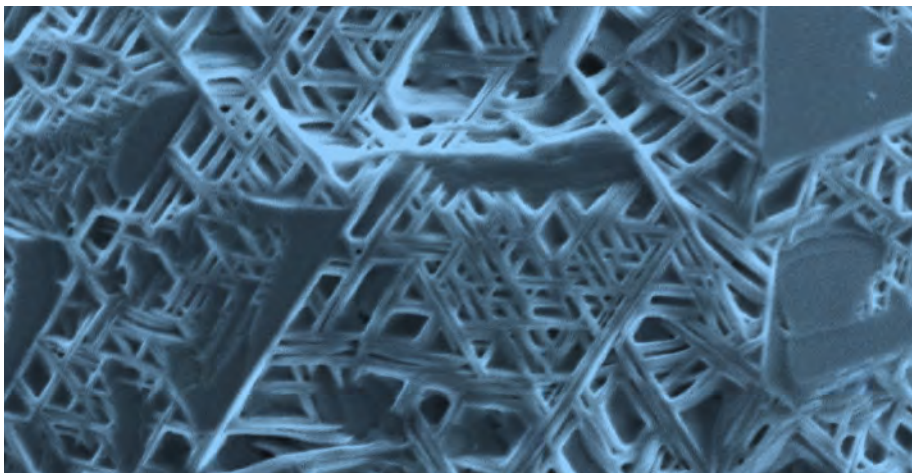
Programme: Training University Lecturers (FPU)
Period: 2016-2020
Funding Institution: Spanish Ministry of Education, Culture and Sport
B. Bellón

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

2.3. Regional

Programme: Talent Atraction Programme – Modality 2
Period: 2018-2022
Funding Institution: Madrid Regional Government
Dr. M. Vila

Programme: Talent Atraction Programme – Modality 2
Period: 2018-2022
Funding Institution: Madrid Regional Government
Dr. A. Orozco



Programme: Talent Atraction Programme – Modality 2
Period: 2018-2022
Funding Institution: Madrid Regional Government
Dr. I. Papadimitriou

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 / 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. D. Iglesias, E. Senokos, B. Alemán, L. Cabana, C. Navio, R. Marcilla, M. Prato, J. J. Vilatela and S. Marchesan. *Gas-phase functionalization of macroscopic carbon nanotube fiber assemblies: reaction control, electrochemical properties, and use for flexible supercapacitors.* **ACS App. Mater. Interf. 10**, 5760, 2018.
2. Afshin Pendashteh, Jesus Palma, Marc Anderson, Juan J. Vilatela and Rebeca Marcilla. *Doping of Self-Standing CNT Fibers: Promising Flexible Air-Cathodes for High-Energy-Density Structural Zn–Air Batteries* **ACS Applied Energy Materials 1**, 2434, 2018.
3. A. Cherevan, P. Gebhardt, A. Kunzmann, R. D. Costa and D. Eder. *Beware of doping: Ta2O5 nanotube photocatalyst using CNTs as hard templates.* **ACS Applied Energy Materials 1**, 1259, 2018.
4. O. Langmar, C. R. Ganivet, T. Scharl, G. de la Torre, T. Torres, R. D. Costa and D. M. Guldi. *Modifying the Semiconductor/Electrolyte Interface in CuO p-Type Dye-Sensitized Solar Cells: Optimization of Iodide/Triiodide-Based Electrolytes.* **ACS Applied Energy Materials 1**, 6388, 2018.
5. V. Etacheri, N. Hong, J. Tang and V. G. Pol. *Cobalt Nanoparticles Chemically Bonded to Porous Carbon Nanosheets: A Stable High-Capacity Anode for Fast-Charging Lithium-Ion Batteries.* **ACS Applied Materials & Interfaces 10**, 4652–4661, 2018.
6. M. Rana, S. Mondal, L. Sahoo, K. Chatterjee, P. E. Karthik and U. K. Gautam. *Emerging Materials in Heterogeneous Electrocatalysis Involving Oxygen for Energy Harvesting*. **ACS Applied Materials and Interfaces 10**, 33737-33767, 2018.
7. S. Lepeshov, M. Wang, A. Krasnok, O. Kotov, T. Zhang, H. Liu, T. Jiang, B. Korgel, M. Terrones, Y. Zheng and A. Alú. *Tunable Resonance Coupling in Single Si Nanoparticle-Monolayer WS 2 Structures.* **ACS Applied Materials and Interfaces 10**, 16690-16697, 2018.
8. M. Witman, S. Ling, P. Boyd, S. Barthel, M. Haranczyk, B. Slater and B. Smit. *Cutting materials in half: a graph theory approach for generating crystal surfaces and its prediction of 2D zeolites.* **ACS Central Science 4**, 235-245, 2018.
9. C. Fernández Aguiño, M. Lang, V. Fernández-Luna, M. Pröschel, U. Sonnewald, P. B. Coto and R. D. Costa. *Single-Component Biohybrid Light-Emitting Diodes Using a White-Emitting Fused Protein.* **ACS Omega 3**, 15829, 2018.
10. D. Wang, C. Li, H. Fan, T. Aziz, C. Bittencourt, L. Wu and P. Dubois. *Biobased Epoxy Resin with Low Electrical Permissivity and Flame Retardancy: From Environmental Friendly High-Throughput Synthesis to Properties.* **ACS Sustainable. Chemistry and Engineering 6(7)**, 8856–8867, 2018.

11. S. Haouala, J. LLorca and J. Segurado. *An analysis of the influence of grain size on the strength of FCC polycrystals by means of computational homogenization.* **Acta Materialia 148**, 72-85, 2018.
12. A. Pineau, G. Guillemot, D. Tourret, A. Karma and Ch. A. Gandin. *Growth competition between columnar dendritic grains - Cellular Automaton versus Phase-Field modeling.* **Acta Materialia 155**, 286-301, 2018.
13. L. W. Yang, C. R. Mayer, N. Li, J. K. Baldwin, N. A. Mara, N. Chawla, J. M. Molina-Aldareguía and J. LLorca. *Mechanical properties of metal-ceramic nanolaminates: effect of constraint and temperature.* **Acta Materialia 142**, 37-48, 2018.
14. Y. Song, D. Tourret, F. L. Mota, J. Pereda, B. Billia, N. Bergeon, R. Trivedi and A. Karma. *Thermal-field effects on interface dynamics and microstructure selection during alloy directional solidification.* **Acta Materialia 150**, 139-152, 2018.
15. C. M. Cepeda-Jiménez, C. Prado-Martínez and M.T. Perez-Prado. *Understanding the high temperature reversed yield asymmetry in a Mg-rare earth alloy by slip trace analysis.* **Acta Materialia 145**, 264-277, 2018.
16. L. W. Yang, C. Mayer, N. Li, J. K. Baldwin, N. A. Mara, N. Chawla, J. M. Molina-Aldareguia and J. LLorca. *Mechanical properties of metal-ceramic nanolaminates: Effect of constraint and temperature.* **Acta Materialia 142**, 37-48, 2018.
17. X. L. Li, R. Wang, C. F. Yang, Z. F. Dong, X. Q. Zhang, D. J. Wang and D. Y. Wang. *Effect of poly (D-lactic acid) block copolymers with soft chains on the tensile behavior of poly(L-lactic acid).* **Acta Polymerica Sinica 5**, 598-606, 2018.
18. N. Ur Rahman, L. Capuano, A. Van der Meer, M. B. de Rooij, D. T. A. Matthews, G. Walmag, M. Sinnaeve, A. García-Junceda, M. Castillo and G.R.B.E. Römer. *Development and characterization of multilayer laser cladded high speed steels.* **Additive Manufacturing 24**, 76-85, 2018.
19. A. Kunzmann, S. Valero, A. E. Sepúlveda, M. Rico-Santacruz, E. Lalinde, J. R. Berenguer, J. García-Martínez, D. M. Guldi, E. Serrano and R. D. Costa. *Hybrid dye-titania nanoparticles for superior low-temperature dye-sensitized solar cells.* **Advanced Energy Materials 8**, 1702583, 2018.
20. R. D. Costa. *Bio-materials for Light Management.* **Advanced Functional Materials 28**, 1802462, 2018.
21. E. Fresta, V. Fernández-Luna, P. B. Coto and R. D. Costa. *Merging Biology and Solid-State Lighting: Recent Advances in Light-Emitting Diodes Based on Biological Materials.* **Advanced Functional Materials 28**, 1707011, 2018.
22. M. D. Weber, E. Fresta, M. Elie, M. E. Miehlich, J. L. Renaud, K. Meyer, S. Gaillard and R. D. Costa. *Rationalizing fabrication and design towards highly efficient and stable blue light-emitting electrochemical cells based on NHC copper(I) complexes.* **Advanced Functional Materials 28**, 1707423, 2018.
23. C. Chen, J. F. M. Oudenhoven, D. L. Danilov, E. Vezhlev, L. Gao, N. Li, F. M. Mulder, R. A. Eichel and P. H. L. Notten. *Origin of Degradation in Si-Based All-Solid-State Li-Ion Microbatteries.* **Advanced Energy Materials 8**, 1801430, 2018.

24. M. C. Demirel, M. Vural and M. Terrones. *Composites of Proteins and 2D Nanomaterial*. **Advanced Functional Materials 28**, 1704990, 2018.
25. M. Wang, A. Krasnok, T. Zhang, L. Scarabelli, H. Liu, Z. Wu, L. M. Liz-Marzán, M. Terrones, A. Alù and Y. Zheng. *Tunable Fano Resonance and Plasmon–Exciton Coupling in Single Au Nanotriangles on Monolayer WS2 at Room Temperature*. **Advanced Materials 30**, 1705779, 2018.
26. J. Segurado, R. A. Lebensohn, J. LLorca. *Computational homogenization of polycrystals.* **Advances in Applied Mechanics 51**, 1-114, 2018.
27. V. Fernández-Luna, P. B. Coto, R. D. Costa. *When fluorescent proteins meet white light-emitting diodes.* **Angewandte Chemie International 57**, 8826, 2018.
28. F. E. Merrill, J. Goett, J. W. Gibbs, S. D. Imhoff, F. G. Mariam, C. L. Morris, L. P. Neukirch, J. Perry, D. Poulson, R. Simpson, P. L. Volegov, P. L. Walstrom, C. H. Wilde, C. Hast, K. Jobe, T. Smith, U. Wienands, A. J. Clarke, D. Tourret. *Demonstration of Transmission High Energy Electron Microscopy.* **Applied Physics Letters 112**, 144103, 2018.
29. X. Zhang, L. Yang and H. Liu. *High-temperature conduction behavior of carbon nanotube fiber from 25 °c to 1100 °c*. **Applied Physics Letters 112**, 164103, 2018
30. H. Dong, J. Wang, G. Xu, L. Zhou and Y. Cui. *Assessment of atomic mobility for BCC Ti-Mn and Ti-Al-Mn alloys*. **Calphad: Computer Coupling of Phase Diagrams and Thermochemistry 62**, 141-147, 2018.
31. W. Zheng, J. Wang, Y. He, X. G. Lu, L. Li. *Experimental and computational study of diffusion mobilities for the bcc phase in the Fe-Al-(Si, Mn) systems*. **Calphad: Computer Coupling of Phase Diagrams and Thermochemistry 61**, 189-197, 2018.
32. S. Mao, C. Wang, N. Li, J. Wang, Y. Chen, G. Xu, Y. Guo, Y. Cui. *Kinetic diffusion multiple: A high throughput approach to screening the composition-microstructure-micromechanical properties relationships*. **Calphad: Computer Coupling of Phase Diagrams and Thermochemistry 61**, 219-226, 2018.
33. A. Monreal-Bernal, J. J. Vilatela and R. D. Costa. *CNT fibres as dual counter-electrode/current-collector in highly efficient and stable dye-sensitized solar cells.* **Carbon 141**, 488, 2018.
34. J. C. Fernandez, B. Aleman, A. Ridruejo and J. J. Vilatela. *Tensile properties of carbon nanotube fibres described by the fibrillar crystallite model.* **Carbon 133**, 44, 2018.
35. A. Bianco, Y. Chen, D. Ghoshal, R. H. Hurt, Y. A. Kim, N. Koratkar, V. Meunier and M. Terrones. *A carbon science perspective in 2018: Current achievements and future challenges.* **Carbon 132**, 785-801, 2018.
36. V. J. González, S. M. Vega-Díaz, A. Morelos-Gómez, K. Fujisawa, M. Endo, O. M. Cadiz, J. B. Llido and M. Terrones. *H2O2/UV layer-by-layer oxidation of multiwall carbon nanotubes: The "onion effect" and the control of the degree of surface crystallinity and diameter*. **Carbon 139**, 1027-1034, 2018.

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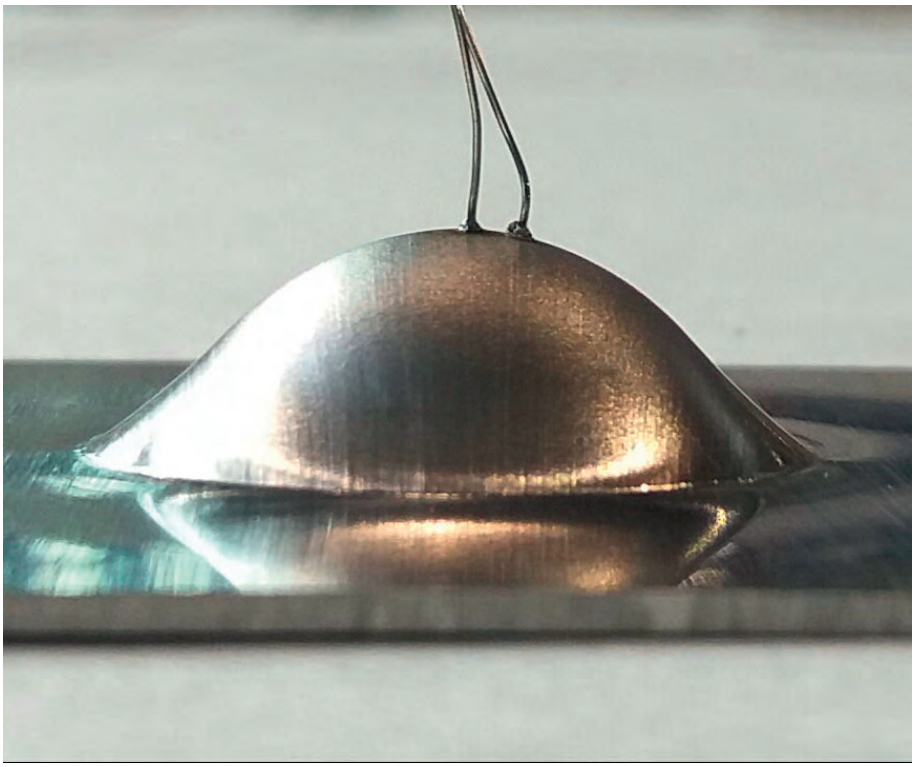
38. D. Banerjee, C. Simon, E. Sameh, M. Haranczyk and P. Thallapally. *Xenon Gas Separation and Storage using Metal Organic Frameworks.* **Chem 4**, 466-494, 2018.
39. M. Bidikoudi, E. Fresta and R. D. Costa. *White-emitting perovskite based lighting devices.* **Chem Commun 54**, 8150, 2018.
40. A. Burger, A. Kunzmann, R. D. Costa, R. Srikantharajah, W. Peukert, D. M. Guldi and A. Hirsch. *Cover: Synergy of Catechol-Functionalized Zinc Oxide Nanorods and Porphyrins in Layer-by-Layer Assemblies.* **Chemistry: A European Journal 24**, 7883, 2018.
41. A. Burger, A. Kunzmann, R. D. Costa, R. Srikantharajah, W. Peukert, D. M. Guldi and A. Hirsch. *Synergy of Catechol-Functionalized Zinc Oxide Nanorods and Porphyrins in Layer-by-Layer Assemblies.* **Chemistry: A European Journal 24**, 7896, 2018.
42. J. Fernandez-Cestau, L. Rocchigiani, A. Pintus, R. J. Rama, P. H. M. Budzelaar and M. Bochmann. *Isocyanide insertion into Au-H bonds: First gold iminoformyl complexes*. **Chemical Communications 54**, 11447-11450, 2018.
43. H. Yue, J. Guo, S. Fu, X. Li, W. Wen, W. Jiang, R. Tong, R. Wang and M. Haranczyk. *Structural design, preparation and characteirzation of light, isotropic and robust statically determined organic frameworks.* **Chemical Engineering Journal 335**, 887-895, 2018.



44. Y. T. Pan, C. Trempont and D. Y. Wang. Corrigendum to *"Hierarchical nanoporous silica doped with tin as novel multifunctional hybrid material to flexible poly (vinyl chloride) with greatly improved flame retardancy and mechanical properties"*. **Chemical Engineering Journal 345**, 707, 2018.
45. Y. T. Pan, J. Wan, X. Zhao, C. Li and D. Y. Wang. *Corrigendum to "Interfacial growth of MOF-derived layered double hydroxide nanosheets on graphene slab towards fabrication of multifunctional epoxy nanocomposites"*. **Chemical Engineering Journal 345**, 706, 2018.
46. R. Mercado, R. S. Fu, A. Yakutovich, L. Talriz, M. Haranczyk and B. Smit. *In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications.* **Chemistry of Materials 30**, 5069-5086, 2018.
47. J. Düring, A. Kunzmann, M. S. Killian, R. D. Costa, D. M. Guldi and F. Gröhn. *Porphyrins as Multifunctional Interconnects in Networks of ZnO Nanoparticles and their Application in Dye-Sensitized Solar Cells.* **ChemPhotoChem 2**, 213, 2018.
48. A. Monreal-Bernal and J. J. Vilatela. *Large Area Schottky Junctions between ZnO and CNT Fibres.* **ChemPlusChem 83**, 285, 2018.
49. P. B. Coto and R. D. Costa. *New Materials and Approaches for Advanced Optoelectronics.* **ChemPlusChem 83**, 144, 2018.
50. A. Charisiadis, A. Bagaki, E. Fresta, K. T. Weber, G. Charalambidis, C. Stangel, A. G. Hatzidimitriou, P. A. Angaridis, A. G. Coutsolelos and R. D. Costa. *Peripheral substitution of tetraphenyl porphyrins: Fine-tuning self-assembly for enhanced electroluminescence.* **ChemPlusChem 23**, 254, 2018.
51. O. Falcó, R. L. Ávila, B. Tijs and C. S. Lopes. *Modelling and simulation methodology for unidirectional composite laminates in a Virtual Test Lab framework.* **Composite Structures 190**, 137–159, 2018.
52. W. Tan, F. Naya, T. Chang, L. Yang, B. G. Falzon, L. Zhan, J. Molina, C. Gonzáleza and J. LLorca. *The role of interfacial properties on the intralaminar and interlaminar damage behaviour of unidirectional composite laminates: experimental characterization and multiscale modelling.* **Composites B 138**, 206-221, 2018.
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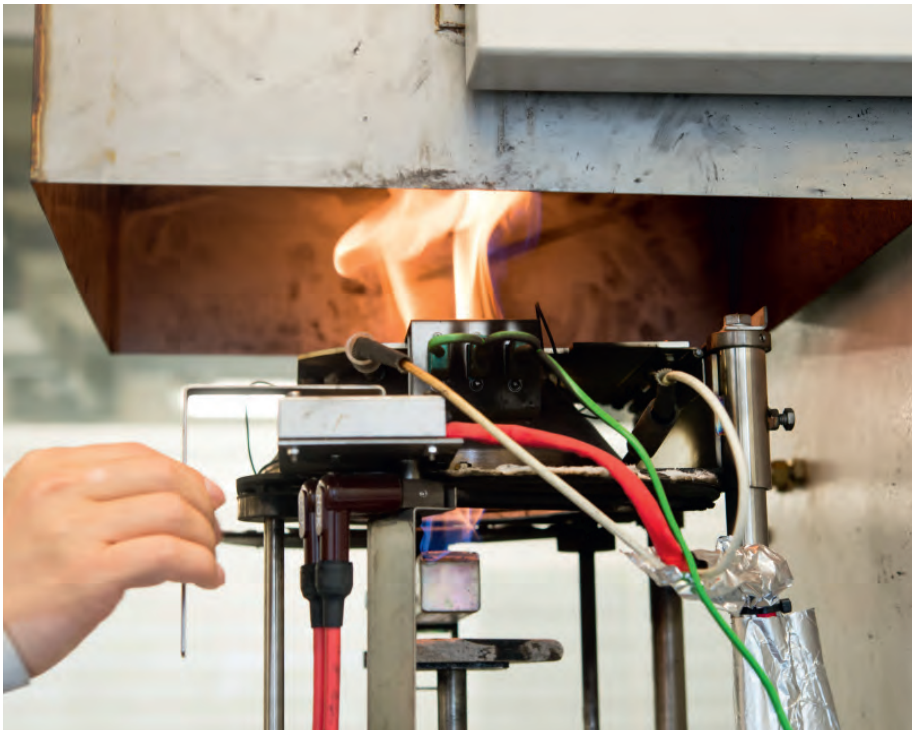

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3.2. Book chapters

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3.3. Patent applications

1. *Improvements Relating to Thermoelectric Materials.* University of Limerick and IMDEA Materials Institute. Patent application number 1820651.6 (18 December 2018).

3.4. Software registered

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3.5. International conferences

Invited and plenary talks

1. *"A roadmap for multiscale modelling of processing and properties of metallic alloys*", J. LLorca, **1st Manufacturing using Advanced Powder Processes International Conference**, Sheffield, U. Kingdom, January 2018.
2. *"White Hybrid Light-Emitting Diodes*", R. D. Costa, **International Workshop in Materials and Optoelectronics,** Tokyo, Japan, February 2018.
3. *"Deformation mechanism map of Cu/Nb nanoscale metallic multilayers as a function of temperature and layer thickness*", J. Molina-Aldareguia, **DPG Spring Meeting**, Berlin, Germany, March 2018.

4. *"Deformation mechanisms of Cu/Nb nanoscale metallic multilayers as a function of temperature and layer thickness*", M. Monclus, J. Snel, M. Castillo-Rodriguez, N. Mara, I. J. Beyerlein, J. LLorca, J. M. Molina-Aldareguia, **TMS 2018: Annual Meeting & Exhibition of the The Minerals, Metals & Materials Society**, Phoenix, USA, March 2018.
5. *"Effects of layer thickness on the mechanical behavior of oxidation strengthened Zr/Nb nanoscale multilayers*", J. M. Molina-Aldareguia, M. Monclús, M. Callisti, T. Polcar, L. Yang, J. LLorca, **TMS 2018: Annual Meeting & Exhibition of the The Minerals, Metals & Materials Society**, Phoenix, USA, March 2018.
6. "*Understanding the role of interfaces on fully lamellar TiAl alloys through micromechanical testing*", J. Molina-Aldareguia, M. Monclús, **TMS 2018: Annual Meeting & Exhibition of the The Minerals, Metals & Materials Society**, Phoenix, USA, March 2018.
7. *"Nanostructured fibres and fabrics for structural supercapacitors*", J. J. Vilatela, **Nanospain**, Bilbao, Spain, March 2018.
8. *"Dislocation propagationnano across lamellar boundaries in fully lamellar TiAl alloys: insights from micro-tensile experiments*", J. Molina-Aldareguia, **Symposium on Fine-Scale Mechanical Characterization and Behavior**, Cambridge, UK, April 2018.
9. *"Structural energy storage in transport*", J. J. Vilatela, **Plastics are Future**, Valencia, Spain, April 2018.
10. *"An atomistic investigation of the interaction of dislocations with Guinier-Preston zones in Al-Cu alloys*", G. Esteban-Manzanares, E. Martínez, J. Segurado, J. LLorca, **38th CNLS Annual Conference –Rate-Theory and Long Timescale Simulations**, Santa Fe, Mexico, May 2018.
11. *"CNT fibre electrodes for energy storage and conversion*", J. J. Vilatela, **Nanotechnology Materials and Devices (NMD) Workshop**, Cincinnati, USA, May 2018.
12. "*Pseudocapacitance assisted Li and Na ion storage in transition metal oxide nanostructures*", V. Etacheri, **Nanotech conference 2018**, Rome, Italy, May 2018.
13. *"A new thermodynamically consistent finite element method for compressible flow*", D. Portillo, I. Romero, **6th European Conference on Computational Mechanics**, Glasgow, Scotland, June 2018.
14. *"Variational updates for strongly coupled thermomechanical problems including mass transport",* E. M. Andrés, A. Ortiz-Toranzo, I. Romero, **6th European Conference on Computational Mechanics**, Glasgow, Scotland, June 2018.
15. *"Deformation mechanisms of fully lamellar TiAl alloys studied by micromechanical testing*", J. Molina-Aldareguia, **Workshop on Micromechanical Properties of Hard Materials**, Barcelona, Spain, June 2018.
16. *"Proteinas fluorescentes en nuestras luces ¿el futuro de una iluminacion ecológica y saludable?",* R. D. Costa, **II Jornadas de Química para profesores de Secundaria**, Valencia, Spain, June 2018.
17. "*Multiscale modelling of precipitation hardening in Al-Cu alloys*", J. LLorca, **Micromechanics of Defects in Crystalline Solids and Metals**, Sevilla, Spain, June 2018.

18. *"Nanocarbon fabrics for energy storage in structural composites*", J. J. Vilatela, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
19. *"Precipitation in Al-Cu alloys: A multiscale analysis based on first principles calculations*", J. LLorca, **10 Years ICAMS International Symposium**, Bochum, Germany, June 2018.
20. *"Nano fire retardant to polymers: Where we are and where we go".* D.-Y. Wang. **5th International Symposium on Flame-Retardant Materials & Technologies (ISFRMT2018).** Hangzhou, China, June 2018.
21. *"Functionalization of nanomaterials vs fire behavior of polymers".* D.-Y. Wang. **5th International Conference on Multi-Functional Materials and Structures (MFMS2018),** Shenyang, China, June 2018.
22. *"A numerical framework to analyze fracture in composite materials: from simulated crack resistance curves to homogenized softening laws*", M. Herráez, C. González, C. S. Lopes, **13th World Congress on Computational Mechanics (WCCM2018)**, New York, USA, July 2018.
23. *"Design of aluminium alloys suitable for additive manufacturing*", C. M. Cepeda-Jiménez, A. Martin, M. Cejuela, S. Milenkovic, M. T. Pérez-Prado, **THERMEC'18- Intl' Conf. on Processing & Manufacturing of Advanced Materials**, Paris, France, July 2018.
24. *"Why can´t Mg alloys be strengthened by precipitation?*", C. M. Cepeda-Jiménez, M. T. Pérez-Prado, **THERMEC'18- Intl' Conf. on Processing & Manufacturing of Advanced Materials**, Paris, France, July 2018.
25. *"Effect of grain size on the strength of FCC polycrystals: strain gradient and mean free path contributions*", S. Haouala, S. Lucarini, J. Segurado, J. LLorca, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
26. *"High temperature performance of metallic nanoscale multilayers*", J. LLorca, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.

27. *"CNT fibres for energy storage and solar conversion",* R. D. Costa, **First International Workshop on Multifunctional Nanocarbon Fibres (MNF2018)**, Madrid, Spain, July 2018.
28. *"Effect of processing parameters on the reaction kinetics of Fe-Al intermetallics studied by combined in-situ synchrotron radiography and diffraction*", F. Sket, S. Djaziri, A. Hynowska, S. Milenkovic, **XIV Congreso Nacional de Materiales (CNMAT2018)**, Salamanca, Spain, July 2018.
29. *"Understanding the role of interfaces on the deformation of fully lamellar TiAl alloys through micromechanical testing* ", J. Molina-Aldareguia, **XIV Congreso Nacional de Materiales 2018 (CNMAT2018)**, Salamanca, Spain, July 2018.
30. *"Effect of processing parameters on the reaction kinetics of Fe-Al intermetallics studied by combined in-situ synchrotron radiography and diffraction*", F. Sket, S. Djaziri, A. Hynowska, S. Milenkovic, S. Jana, **XIV Congreso Nacional de Materiales 2018 (CNMAT2018)**, Salamanca, Spain, July 2018.
31. *"Integration schemes that preserve the two laws of thermodynamics for dissipative problems*", D. Portillo, I. Romero, **8th International Workshop on nonequilibrium thermodynamics IWNET**, Sint Michielsgestel, The Netherlands, July 2018.
32. *"Multiscale modelling of composites: Towards virtual testing*", C. González, **4th International Conference on Mechanics of Composites 2018 (MECHCOMP 2018)**, Madrid, Spain, July 2018.
33. *"New advances in physical simulation of metallurgical processes*", I. Sabirov, **International Conference on Materials Manufacturing and Processing**, Xian, China, July 2018.
34. *"Understanding reversed yield asymmetry in Magnesium alloys*", C. M. Cepeda-Jiménez, M. T. Pérez-Prado, **The 11th International Conference on Magnesium Alloys and Their Applications (Mg2018)**, Old Windsor, UK, July 2018.
35. *"Understanding precipitation hardening and mechanical properties in Mg alloys by slip trace analysis and TEM characterization*", C. M. Cepeda-Jiménez, M. T. Pérez-Prado, **XXVII International Materials Research Congress (IMRC 2018)**, Cancún, Mexico, August 2018.
36. *"Effect of processing parameters on the reaction kinetics of Fe-Al intermetallics studied by combined in-situ synchrotron radiography and diffraction*", F. Sket, S. Djaziri, A. Hynowska, S. Milenkovic, **Materials Science and Engineering Congress (MSE 2018)**, Darmstadt, Germany, September 2018.
37. *"Combined synchrotron radiography and diffraction for in situ study of reactive infiltration of Al into Fe porous preform*", F. Sket, S. Djaziri, A. Hynowska, S. Milenkovic, **Materials Science and Engineering Congress (MSE 2018)**, Darmstadt, Germany, September 2018.
38. *Effect of ultrafast heating on properties of a low carbon steel on macro- and micro-scales*", M. A. Valdes-Tabernero, F. Vercruysse, R. Petrov, M. A. Monclus, J. M. Molina-Aldareguia, I. Sabirov, **Materials Science and Engineering Congress (MSE 2018)**, Darmstadt, Germany, September 2018.
39. *"A quantitative benchmark of multiscale models for dendritic growth*", D. Tourret, **Solidification & Gravity '18**, Miskolc- Lillafüred, Hungary, September 2018.

40. *"A roadmap for multiscale modelling of processing and properties of metallic alloys*", J. LLorca, **AME Programmatic Structural Metal Alloys Scientific Workshop**, Singapore, Singapore, September 2018.
41. *"An extension of the Kobayashi–Warren–Carter model to the five-dimensional grain boundary space*", J. Segurado, N. Chandra Admal, J. Marian, **Microstructure & Property Relationship of Polycrystalline Materials: Characterization and Modelling**, Santa Fe, Mexico, September 2018.
42. *"Understanding the effect of grain boundaries on polycrystal deformation*", J. LLorca, **Microstructure & Property Relationship of Polycrystalline Materials: Characterization and Modelling**, Santa Fe, Mexico, September 2018.
43. *"Defect and interface induced Li/Na-ion storage in nanoengineered electrodes* ", V. Etacheri, **Battery-Tech Conference 2018**, London, United Kindom, September 2018.
44. *"Nuevos materiales para fabricación aditiva*", M. T. Pérez-Prado, **The 3D printing day**, Campus Google, Madrid, Spain, September 2018.
45. *"From jellyfish to light-emitting diodes"***,** R. D. Costa, **World Economic Forum**, Tianjin, China, September 2018.
46. *"Deformation and fracture mechanisms of nanoscale metallic and metal-ceramic multilayers* ", J. Molina-Aldareguia, **EuroPM Congress & Exhibition (EuroPM 2018)**, Bilbao, Spain, October 2018.
47. *"Facilitating discovery of nanoporous materials for energy applications with porosity analysis tools*", M. Haranczyk, **Hot Topics: Shape and Structure of Materials**, Berkeley, C. A., USA, October 2018.
48. *"Microstructure sensitive fatigue in polycrystalline superalloys: Micromechanical analysis and upscaling from RVEs to full specimens*", J. Segurado, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
49. *"Advanced micromechanical testing techniques applied to hard coatings to measure strength and fracture properties*", J. Molina-Aldareguia, **LVI Congreso Nacional de la SECV**, Barcelona, Spain, October 2018.
50. *"Stabilizing fluorescent proteins in industrial polymer matrices for lighting and photovoltaic applications",* C. Fernandez, R. D. Costa, **Chemplast**, Madrid, Spain, November 2018.
51. *"White hybrid light-emitting diodes",* R. D. Costa, **Energy and Nanomaterials Workshop**, Tokyo, Japan, November 2018.
52. *"Nanocarbon fabrics: an enabler of integrated energy and sensing in aerospace structures*", J. J. Vilatela, **Airbus CNT/Graphene day**, Toulouse, France, November 2018.
53. *"Advanced micromechanical testing techniques applied to hard coatings to measure strength and fracture properties*", J. Molina-Aldareguia, **Advanced nano-mechanical techniques for academic and industrial research**, Aachen, Germany, December 2018.
54. *"New trends in light-emitting electrochemical cells***",** R. D. Costa, **12th SPSJ International Polymer Conference (IPC2018***)*, Hiroshima, Japan, December 2018.
55. *"Grain boundaries: Better understanding their formation in solidification to better control mechanical properties of polycrystalline materials*", D. Tourret, **CNRS-**

Solidification of Metallic Alloys Annual Meeting (Journées Annuelles GdR SAM), Lille, France, December 2018.

56. *"Influence of elemental additions to the microstructure and performance of CoCrFeNi High Entropy Alloy family*", I. Toda-Caraballo, D. San Martín1, H. Valles, M. Valcarcel, S. Milenkovic , T. Pérez Prado, C. Capdevila, **The 2nd International Conference on High-Entropy Materials (ICHEM 2018)**, Jeju, South Corea, December 2018.

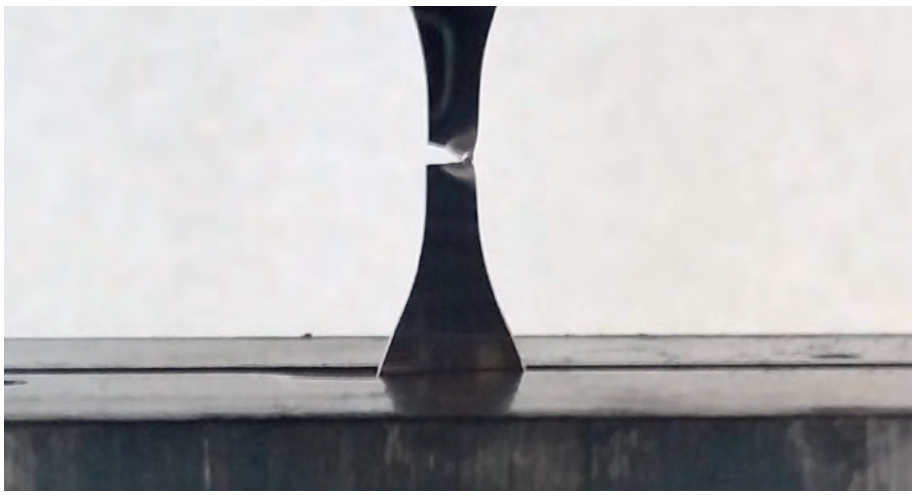
Regular contributions

1. *"Development of a mesoscale finite element constitutive model for fiber kinking*", A. Bergan, M. Herráez, C. González, C. S. Lopes, **2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, AIAA Science and Technology Forum and Exposition 2018**, Gaylord Palms, Kissimmee, Florida, USA, January 2018.
2. *"Organometallo-silica nanoparticles for hybrid inorganic/organic white light-emitting diodes (WHLEDS)",* C. Ezquerro, E. Fresta, R. D. Costa, J. R. Berenguer, J. García-Martínez, **ChemPhys**, Blankenberge, Belgium, February 2018.
3. *"An analysis of the effect of Al content on the critical resolved shear stress for basal slip in Mg by means of micropillar compression*", J. Wang, J. M. Molina-Aldareguia, J. LLorca., **16th European Mechanics of Materials Conference**, Nantes, France, March 2018.
4. *"An atomistic strategy to determine the activation energy for dislocation interaction with Guinier-Preston zones in Al-Cu alloys*", G. Esteban-Manzanares, E. Martínez, J. Segurado, J. LLorca, **16th European Mechanics of Materials Conference**, Nantes, France, March 2018.
5. *"An experimental analysis of the effect of precipitate strengthening on the mechanical response of Al-Cu alloys by means of micropillar compression*", B. Bellón, A. Rodríguez-Veiga, I. Sabirov, J. LLorca, **16th European Mechanics of Materials Conference**, Nantes, France, March 2018.
6. *"Computational micromechanics and homogenization of anisotropic polyurethane foams*", M. Marvi-Mashhadi, C. S. Lopes, J. LLorca, **16th European Mechanics of Materials Conference**, Nantes, France, March 2018.
7. *"Discrete dislocation dynamics simulations of precipitation hardening in Al-Cu alloys*", R. Santos, L. Capolungo, J. Segurado, J. LLorca, **16th European Mechanics of Materials Conference**, Nantes, France, March 2018.
8. *"Multiscale dendritic needle network model for dendritic solidification with liquid convection*", D. Tourret, **TMS 2018: Annual Meeting & Exhibition of the The Minerals, Metals & Materials Society**, Phoenix, USA, March 2018.
9. *"Understanding the role of interfaces on fully lamellar TiAl alloys through micromechanical testing*", J. M. Molina-Aldareguia, A. J. Palomares-García, M. T.

Pérez-Prado **TMS 2018: Annual Meeting & Exhibition of the The Minerals, Metals & Materials Society**, Phoenix, Arizona, USA, March 2018.

10. *"Three-dimensional grain-boundary instability and solitary cell dynamics during directional solidification of binary alloys*", K. Ji, Y. Song, F. L. Mota, D. Tourret, J. Pereda, B. Billia, R. Trivedi, N. Bergeon, A. Karma, **NUconvergence 2018: Frontiers in Aerospace Materials**, Boston, MA, USA, May 2018.
11. *"A numerial framework to analyze fracture in composite materials: from simulated crack resistancre curves to homogenized softening laws*", M. Herráez, C. González, C. S. Lopes,**18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
12. *"A Virtual Test Lab for Unidirectional Composite Coupons*", O. Falcó, B. Tijs, B. Romano, C. S. Lopes, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
13. *"An in-situ investigation of void generation and transport during resin transfer moulding by means of synchrotron X.-Ray laminography*", J. Castro, L- Helfen, C. González, F.Sket, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
14. *"Characterization of elastic and resistance behaviours of 3D printed continuous carbon fibre reinforced thermoplastics*", M. Iragi, C. Pascual-Gonzalez, A. Esnaola, J. Aurrekoetxea, C. S. Lopes, L. Aretxabaleta, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
15. *"Dynamic characterization of Intelaminar toughness in carbon fibre epoxy composite laminates*", M.A. Riezzo, MN. Simmons, C. González, F. Sket, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
16. *"Low-Velocity Impact Simulation of a Woven Composite from a Bottom-Up Multiscale Modelling Strategy*", J. I. Múgica, M. Herráez, F. Naya, C. S. Lopes, C. D. Gonzalez, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
17. *"Recycled basalt fibres: fracture toughness evaluation and strength regeneration*", J. Tirillò, F. Sarasini, L. Di Fausto, C. Gonzalez, A. Fernandez, C. S. Lopes, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
18. *"Recycling of composites by recovering carbon fibers from prepregs and their use*", A. Fernández, C. González, F. López, J. Molina-Aldareguia, C. S. Lopes, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
19. *"Understanding interlaminar toughening mechanisms in structural carbon fiber/epoxy composites interleaved with CNT veils*", Y. Ou, C. González, J. J. Vilatela, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.
20. *"Virtual testing of thermoplastic composites: towards a hybrid simulation-physical testing pyramid*", B. Tijs, C. S. Lopes, A. Turon, C. Bisagni, J. Waleson, J. W. Van Ingen, S. L. Veldman, **18th European Conference on Composite Materials (ECCM18)**, Athens, Greece, June 2018.

21. *"Dynamic contact for finite element method and meshless interaction*", D. Del Pozo, I. Romero, **6th European Conference on Computational Mechanics**, Glasgow, Scotland, June 2018.
22. *"Hybrid white light-emitting diodes (WHLEDS) based on organometallo-silica nanoparticles",* C. Ezquerro, E. Fresta, R. D. Costa, J. R. Berenguer, **EMRS Spring**, Strasbourg, France, June 2018.
23. *"Micromechanical study of crack nucleation and propagation in Ni-based superalloys*", M. Jiménez, J. Molina-Aldareguia, **EMRS Spring**, Strasbourg, France, June 2018.
24. *"In-situ determination of the influence of composition and test-temperature on the damage accumulation of AlSi piston alloys*", K. Bugelnig, F. Sket, H. Germann, T. Steffens, J. Andrien, E. Boller, F. Wilde, G. Requena, **ICAA16**, Montreal, Canada, June 2018.
25. *"Multifunctional polymer composites with metal-organic framework",* X.-L. Qi, **5th International Conference on Multi-Functional Materials and Structures (MFMS2018),** Shenyang, China, June 2018.
26. *"Controllable release: an efficient fire-retardant strategy to polymers",* Z. Li, **5th International Conference on Multi-Functional Materials and Structures (MFMS2018),** Shenyang, China, June 2018.
27. *"Design and study of multifunctional flame retardant polyester fabrics",* C. Fu, **5th International Conference on Multi-Functional Materials and Structures (MFMS2018),** Shenyang, China, June 2018.
28. *"Smoke suppression mechanism of ferrocene-based polymer composites: from vapor-phase to condensed-phase".* Z. Li, **5th International Symposium on Flame-Retardant Materials & Technologies (ISFRMT2018),** Hangzhou, China, June 2018.
29. *"Functional nanomaterial: an interesting way to flame retardant fabric with reduced carbon monoxide release and improved self-cleaning property".* C. Fu, **5th International**



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30. *"Analysis of longitudinal tensile failure of unidirectional composites by means of computational micromechanics*", M. Barzegar, F. Montas, C. S. Lopes, Cláudio, C. Gonzalez, J. Costa, **4th International Conference on Mechanics of Composites (MECHCOPMP 2018)**, Madrid, Spain, July 2018.
31. *"Development of efficient approaches to simulate Compression After Impact strength of composite laminates*", A. H. Baluch, O. Falcó, C. S. Lopes, B. Tijs, **4th International Conference on Mechanics of Composites (MECHCOPMP 2018)**, Madrid, Spain, July 2018.
32. *"Effect of and strength regeneration treatments on the mechanical performance of basalt fibres*", J. Tirillò, F. Sarasini, L. Di Fausto, C. Gonzalez, A. Fernandez, C. S. Lopes, **4th International Conference on Mechanics of Composites (MECHCOPMP 2018)**, Madrid, Spain, July 2018.
33. *"A microstructure informed thermo-visco-plastic constitutive model for ferrite-pearlite steel*", J. Li, J. Segurado, I. Romero, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
34. *"A SPH modelling approach for physics and solid mechanics of engineering applications*", A. Ma, D. Tourret, J. LLorca, J. Segurado, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
35. *"Enhanced strain rate sensitivity of nanotwinned Cu compared to coarse-grained Cu determined by high temperature indentation-creep*", Y. Lingwei, M. Monclús, Ch. Wang, L. Lu, J. Molina-Aldareguia, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
36. *"In-situ micromechanical study of crack nucleation and propagation in Ni-based superalloys*", M. Jiménez, J. Molina-Aldareguia, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
37. *"Novel variational updates for strongly coupled thermomechanical problems including mass transport*", E. M. Andrés, A. Ortiz-Toranzo, I. Romero, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
38. *"Revisiting Gurson-Tvergaard-Needleman model to develop a thermodynamically consistent damage mode*", E. M. Andrés, J. Segurado, I. Romero, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
39. *"Slip transfer at grain boundaries in Al: experimental analysis and numerical simulations*", R. Alizadeh, S. Haouala, T. Bieler, J. Segurado, J. Molina-Aldareguia, J. LLorca, **10th European Solid Mechanics Conference (ESMC18)**, Bologna, Italy, July 2018.
40. *"Study of mechanical properties at the macro- and micro-scale in AHSS processed by ultra-fast heating*", M. Valdés-Tabernero, F. Vercruysse, R. Petrov, I. Sabirov, M. Monclús, J. Molina-Aldareguia, **THERMEC'18- Intl' Conf. on Processing & Manufacturing of Advanced Materials**, Paris, France, July 2018.

41. *"The fatigue behavior of steels processed via quenching and partitioning (Q&P)"*, P. Garcia-Chao, J. Molina-Aldareguia, I. Sabirov, A. Lara, P. Rodriguez-Calvillo, J. Cabrera, **THERMEC'18- Intl' Conf. on Processing & Manufacturing of Advanced Materials**, Paris, France, July 2018.
42. *"Thermo-mechanical physical simulation of friction melt bonding for dissimilar Al/steel joints"*, T. Sapanathan, N. Jimenez-Mena, I. Sabirov, M. Monclús, J. Molina-Aldareguia, A. Simar, **THERMEC'18- Intl' Conf. on Processing & Manufacturing of Advanced Materials**, Paris, France, July 2018.
43. *"Combined synchrotron radiography and diffraction for in situ study of reactive infiltration of Al into Fe porous preform"*, S. Djaziri, F. Sket, A. Hynowska, S. Milenkovic, **ICMSMM 2018**, Barcelona, Spain, August 2018.
44. *"Combined synchrotron radiography and diffraction study of in situ reactive infiltration of Al into Fe porous preform"*, S. Djaziri, F. Sket, S. Milenkovic, A. Hynowska, **EMRS Fall meeting 2018**, Warsaw, Poland, September 2018.
45. *"White-emitting organometallo-silica nanoparticles for sun-like light-emitting diodes",* E. Fresta, R. D. Costa, **EMRS Fall meeting 2018***,* Warsaw, Polland, September 2018.
46. *"Determination of damage mechanisms and damage evolution in fiber metal lamintes containing friction stir welded thin foils"*, U. Alfaro, F. Sket, F. Wilde, G. Requena, **Materials Science and Engineering Congress (MSE 2018)**, Darmstadt, Germany, September 2018.
47. *"In-situ determination of the influence of composition and test-temperature on the damage accumulation of Al-Si piston alloys"*, K. Bugelnig, F. Sket, H. Germann, T. Steffens, J. Adrien, E. Maire, E. Boller, F. Wilde, G. Requena, **Materials Science and Engineering Congress (MSE 2018)**, Darmstadt, Germany, September 2018.
48. *"Ultrafine Fe-Fe2Ti eutectics produced by laser metal deposition: processing and characterization"*, A. Theofilatos, G. Rödler, J. Haubrich, G. Requena, U. Hecht, R. Laqua, A. Weisheit, F. Sket, S. Milenkovic, L. Granay, T. Pusztai, L. Rat, **Materials Science and Engineering Congress (MSE 2018)**, Darmstadt, Germany, September 2018.
49. *"Novel reactive infiltration method for production of fine grained Fe-Al intermetallics"*, S. Milenkovic, **YUCOMAT 2018**, Herceg Novi, Montenegro, September 2018.
50. *"On the use of X-ray tomography to address void distribution and effects in composite materials"*, C. González, J. J. Torres, M. Simmons, F. Sket, **TEXCOMP 13**, Milan, Italy, September 2018.
51. *"Dynamic characterization of interlaminar toughness in carbon fibre epoxy composite laminates"*, M. A. Riezzo, M. Simmons, C. González, F. Sket, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
52. *"A numerical framework to analyze fracture in composite materials: From simulated crack resistance curves to homogenized softening laws"*, M. Herráez, C. González, C.S. Lopes, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.

53. *"A novel variational formulation of the strongly coupled thermomechanical problem including mass transport*", E. M. Andrés, A. Ortiz-Toranzo, J. Segurado, I. Romero, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
54. *"Additive manufacturing of aluminum alloys*", C. Galera, M. Montero-Sistiaga, K. Vanmeensel, M. Godino-Martinez, M. T. Perez-Prado, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
55. *"Advanced virtual characterization of UD composite laminates*", C. S. Lopes, O. Falcó, B. Tijs, S. Sádaba, M. Herráez, C. González, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
56. *"An atomistic investigation of the interaction of dislocations with Guinier-Preston zones in Al-Cu alloys*", G. Esteban-Manzanares, E. Martínez, J. Segurado, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
57. *"An extension of the Kobayashi–Warren–Carter model to the five-dimensional grain boundary space*", J. Segurado, N. Chandra Admal, J. Marian, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
58. *"Effect of orientation on the deformation and fracture mechanisms of Cu/Nb nanolaminates by in-situ TEM mechanical tests*", Z. Liu, M. A. Monclús, L. Yang, M. Castillo-Rodríguez, J. M. Molina-Aldareguia, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
59. *"Composition and microstructural characterisation of fiber filaments and thermosplastic resins used in 3D-printing of continuously reinforced composites*", C. Pascual-González, J. I. Múgica, C. González, C. S. Lopes, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
60. *"Effect of precipitates on the critical resolved shear stress for basal slip in Mg-4 (wt. %) Zn alloy*", R. Alizadeh, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
61. *"Effect of solutes on the plastic deformation of β-Ti alloys: a high throughput investigation*", C. Wang, M. T. Pérez-Prado, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
62. *"Experimental analysis of the effect of Al solid solution on the critical resolved shear stress for basal slip and twinning in Mg as a function of temperature*", D. Wang, J. M. Molina-Aldareguia, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
63. *"Fiber Kinking: From Micro to Mesomechanics*", M. Herráez, C. S. Lopes, C. González, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
64. *"Gleeble simulation of gas atomized γ-TiAl powder microstructure*", A. Martín, C. M. Cepeda-Jimenez, A. J. Palomares-García, I. Sabirov, M. Cejuela, J. M. Molina-Aldareguia, M. T. Pérez-Prado, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.

65. *"High velocity impacts of composite fragments on aluminum plates"*, J.M. Rodríguez-Sereno, J.A. Artero-Guerrero, J López-Puente, J. Pernas-Sánchez, D. Varas, J. Múgica, C. S. Lopes, E. Martino, V. Votsios, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
66. *"Implementation of a parallel multiphysics meshless simulator for complex Engineering problems"*, J. Li, A. Ma, I. Romero, J. Segurado, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
67. *"Mechanical characterization of 3D printed continuous fibre reinforced thermoplastics"*, M. Iragi, L. Aretxabaleta, C. Pascual-Gonzalez, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
68. *"Mechanical properties of recycled fibres and their re-use"*, A. Fernández, C. González, F. López, J. Molina-Aldareguia, C. S. Lopes, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
69. *"Nanoindentation impact testing methodologies for the high strain rate characterization of materials at the microscale"*, M. Rueda-Ruiz, B. D. Beake, J. Molina-Aldareguia, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
70. *"On the effect of stress-free transformation strains and dislocation cross-slip in precipitate strengthening in Al-Cu alloys"*, R. Santos, G. Esteban-Manzanares, L. Capolungo, E. Martínez, J. Segurado, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
71. *"Simulation of slip transfer in tensile deformed bicrystals using a dislocation density based crystal plasticity model"*, S. Haouala, T. R. Bieler, J. Segurado, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
72. *"Solid-Liquid interface properties in the Al-Cu system: A Molecular Dynamics study"*, I. Papadimitriou, G. E. Manzanares, D. Tourret, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
73. *"The effect of nucleating particles on the microstructure and mechanical properties of 3D printed high strength Al alloys"*, C. Galera-Rueda, M. L. Montero-Sistiaga, K. Vanmeensel, M. Godino-Martinez, M. T. Pérez-Prado, J. LLorca, **Society of Engineering Science (SES 2018), 55th Annual Technical Meeting**, Madrid, Spain, October 2018.
74. *"Atomistic and continuum approaches to analyse precipitation hardening in metallic alloys"*, G. Esteban-Manzanares, R. Santos, A. Ma, I. Papadimitriou, E. Martínez, L. Capolungo, J. Segurado, J. LLorca, **9th International Conference on Multiscale Materials Modeling**, Osaka, Japan, October 2018.
75. *"Fast screening of modified powder compositions for selective laser melting"*, M. L. Montero-Sistiaga, M. Deprez, M. Godino-Martínez, C. Hautfenne, A. Martín, M. T. Pérez-Prado, J-P Kruth, K. Vanmeensel, **EuroPM Congress & Exhibition (EuroPM 2018)**, Bilbao, Spain, October 2018.
76. *"Influence of elemental additions to the microstructure and performance of CoCrFeNi High Entropy Alloy family"*, I. Toda-Caraballo, D. San Martín, H. Valles, M. Valcárcel,

S. Milenkovic, M. T. Pérez-Prado, C. Capdevila, **2nd International Conference on High Entropy Materials (ICHEM 2018)**, Jeju, Korea, December 2018.

77. *"Recent developments in prediction, characterization and screening of porous crystalline framework materials*", M. Haranczyk, **6th International Conference on Metal-Organic Frameworks (MOF 2018)**, Auckland, New Zealand, December 2018.

Membership in organising committees

1. **Thermo-mechanical Response of Materials with Special Emphasis on In Situ Techniques - TMS 2018: Annual Meeting & Exhibition of the The Minerals, Metals & Materials Society.** M. T. Pérez-Prado (Symposium organiser). Phoenix, Arizona, USA, March 2018.
2. **Frontiers in Solidification Science and Engineering - TMS 2018: Annual Meeting & Exhibition of the The Minerals, Metals & Materials Society.** M. Asle Zaeem, D. Tourret, M. Eshraghi, J. Hoetzer (Symposium organisers). Phoenix, Arizona, USA, March 2018.
3. **First International Workshop on Multi-functional Nanocarbon Fibres - MNF2018.** J. J. Vilatela, M. Terrones, I. Martín Gullón (Organisers). Madrid, Spain, June 2018.
4. **5th International Conference on Multi-Functional Materials and Structures (MFMS 2018).** D. Y. Wang (Chairman). Shenyang, China, June 2018.
5. **5th International Symposium on Flame-Retardant Materials & Technologies (ISFRMT2018),** D.-Y. Wang (Member of international scientific committee), Hangzhou, China, June 2018.
6. **11th International Conference on Magnesium Alloys and their Applications (Mg2018).** M. T. Pérez-Prado (Member of the scientific committee). Beaumont Estate, UK, July 2018.
7. **Advanced Characterization of Materials - XIV Congreso Nacional de Materiales (CNMAT 2018).** M. T. Pérez-Prado (Symposium organiser). Salamanca, Spain, July 2018.
8. **Summer school and industry day on Additive Manufacturing - DIMMAT R&D project_ Tecnologías 2013 call, Madrid Regional Government.** M. T. Pérez-Prado, S. Milenkovic (Organisers), Madrid, Spain, July 2018.
9. **18th International Conference on the Strength of Materials (ICSMA 18).** M. T. Pérez-Prado (Member of the international advisory board). Ohio, USA, July 2018.
10. **Multiscale Modelling of Polycrystalline Materials – 10th European Solid Mechanics Conference (ESMC18).** J. Segurado, R. Lebensohn (Symposium organisers), Bologna, Italy, July 2018.
11. **Experimental Micromechanics and Nanomechanics - 10th European Solid Mechanics Conference (ESMC18).** G. Dehm, J. Molina-Aldareguia, M. Monclús (Symposium organisers), Bologna, Italy, July 2018.
12. **13th International Conference on Superplasticity in Advanced Materials (ICSAM 2018).** M. T. Pérez-Prado (Member of the international advisory board), St. Petersburg, Russia, August 2018.

13. **55th Annual Technical Meeting of the Society of Engineering Science (SES 2018),** I. Romero, J. LLorca (Chairmen), Madrid, Spain, October 2018.
14. **Phase-Field Methods in Science and Engineering - 55th Annual Technical Meeting of the Society of Engineering Science (SES 2018)**. D. Tourret, A. Karma (Symposium organisers), Madrid, Spain, October 2018.
15. **Additive Manufacturing - 55th Annual Technical Meeting of the Society of Engineering Science (SES 2018).** M. T. Pérez-Prado (Symposium organizer), Madrid, Spain, October 2018.

3.6. Hosting and organisation of international conferences and workshops

One international conference and one international workshop were organised by IMDEA Materials Institute in 2018. Over 700 delegates attended these events, enhancing the international visibility of our activities.

1. **First International Workshop on Multi-functional Nanocarbon Fibres (MNF)**, Dr. J. J. Vilatela, Prof. M. Terrones, Prof. I. Martín Gullón, 27-29 June 2018

In June 2018, IMDEA Materials hosted the First International Workshop on Multi-functional Nanocarbon Fibres. The meeting gathered leading international researchers working on nanocarbons developing the next generation of functional carbon fibres and fabrics based on nanobuilding blocks. During the three day-workshop, over 60 delegates listened fascinating talks about the scientific/technological challenges and opportunities for the use of functional carbon fibres in energy storage, composites, sensors and other applications. This workshop constituted a satellite meeting of the Carbon 2018 Conference, which was be held in Madrid.

2. 55th Annual Technical Meeting of the Society of Engineering Science (SES 2018), Prof. J. LLorca, Prof. I. Romero, 10-12 October 2018

The 55th Society of Engineering Science (SES) Technical Meeting has been held during 54 years in a university campus in North America (with the exception of 1972 in Israel) but this time was hosted by IMDEA Materials Institute in the Leganés (Madrid, Spain) campus of the Carlos III University of Madrid. Bringing this event to Europe has been a bold movement of the Board of Directors of the Society of Engineering Science to spread the goals and objectives of the Society throughout the world.

3.7. Invited seminars and lectures

1. *"Materials engineering: perspectives and trending topics*", J. LLorca, **National Center for Defense Studies (CESEDEN), Minisitry of Defense**, Madrid, Spain, January 2018.
2. *"White bio-hybrid optoelectronics*", R. D. Costa, **Tokyo University of Agriculture and Technology (TUAT)**, Tokyo, Japan, January 2018.
3. *"Materiales metálicos para impresión 3D*", M. T. Pérez-Prado, **GE Industrial Solutions**, Madrid, Spain, February 2018.
4. *"Solidification of alloys and microstructure selection across length and time scales*", D. Tourret, **University of Michigan**, Ann Arbor, MI, USA, February 2018.
5. *"Variational principles and numerical methods coupling nonlinear beams and continua*", I. Romero, **Stanford University**, Stanford, CA, USA, February 2018.
6. *"New advances in physical simulation of metallurgical processes*", I. Sabirov, **Deakin University**, Geelong, Australia, February 2018.
7. *"Multiscale modelling of precipitation hardening in Al-Cu alloys*", J. LLorca, **University of Manchester**, Manchester, U. Kingdom, February 2018.
8. *"Hybrid Optoelectronics*", R. D. Costa, **Carlos III University**, Madrid, Spain, March 2018.
9. *"Coupling beams and continua: Novel variational principles and numerical methods*", I. Romero, **University of Pavia**, Pavia, Italy, April 2018.
10. *"Charge transfer/storage using nanocarbon-based current collector*", J. J. Vilatela, **Autonomous University of Madrid**, Madrid, Spain, April 2018.
11. *"Hybrid Optoelectronics*", R. D. Costa, **IMDEA Nanoscience Institute**, Madrid, Spain, April 2018.
12. *"Understanding Magnesium microplasticity by EBSD-assisted slip trace analysis*", M. T. Pérez-Prado, **Imperial College of London**, London, United Kingdom, May 2018.
13. *"CNT fiber electrodes for energy storage*", J. J. Vilatela, **KTH**, Stockholm, Sweden, May 2018.
14. *"High temperature mechanical properties of metallic and metal-ceramic nanoscale multilayers*", J. LLorca, **Central South University**, Changsha, China, May 2018.

15. *"Multiscale modelling of precipitation hardening in Al-Cu alloys"*, J. LLorca, **Hunan University**, Changsha, China, May 2018.
16. *"Multiscale modelling of precipitation hardening in Al-Cu alloys"*, J. LLorca, **Northwestern University**, Evanston, Illinois, May 2018.
17. *"Multiscale modelling of precipitation hardening in Al-Cu alloys"*, J. LLorca, **University of California Los Angeles**, Los Angeles, California, May 2018.
18. *"Multiscale modelling of precipitation hardening in Al-Cu alloys"*, J. LLorca, **University of California Santa Barbara**, Santa Barbara, California, May 2018.
19. *"Microstructure sensitive fatigue in polycrystalline superalloys: from micromechanics to specimen life prediction"*, J. Segurado, **University of California Santa Barbara**, Santa Barbara, USA, May 2018.
20. *"Advanced nanomechanical testing techniques applied to hard coatings to measure strength and fracture properties"*, J. Molina-Aldareguia, **Swerea KIMAB (Seminar organized by Funmat II)**, Stockholm, Sweden, May 2018.
21. *"Microstructure sensitive fatigue in polycrystalline superalloys: from micromechanics to specimen life prediction"*, J. Segurado, **Los Alamos National Laboratory**, Los Alamos, USA, June 2018.
22. *"Hybrid optoelectronics"*, R. D. Costa, **Amber/Trinity College**, Dublin, Irland, August 2018.
23. *"A computational micromechanics approach to analyze fracture in composite materials and derive homogenized softening laws"*, C. S. Lopes, **Imperial College London**, London, United Kingdom, September 2018.
24. *"A roadmap for the virtual design of metallic materials: from atoms to components"*, J. LLorca, **Institute of High Performance Computing**, Singapore, Singapore, September 2018.
25. *"Multiscale modelling of precipitation hardening in Al-Cu alloys"*, J. LLorca, **Texas A&M University, College Station**, Texas, USA, September 2018.
26. *"Nanoscale engineering of materials and interfaces for high performance rechargeable batteries"*, V. Etacheri, **Polytechnic University Madrid**, Madrid, Spain, September 2018.
27. *"A roadmap for multiscale modelling of processing and properties of metallic materials"*, J. LLorca, **University of Edinburgh**, Edinburgh, U. Kingdom, October 2018
28. *"Hybrid Materials and their new applications"*, R. D. Costa, **Tokyo Institute of Technology**, Tokyo, Japan, November 2018.
29. *"Light-emitting electrochemical cells"*, R. D. Costa, **Waseda University**, Tokyo, Japan, November 2018.
30. *"Hybrid photovoltaics: DSSCs and perovskites"*, R. D. Costa, **Waseda University**, Tokyo, Japan, November 2018.
31. *"Hybrid Light-emitting diodes"*, R. D. Costa, **Waseda University**, Tokyo, Japan, November 2018.
32. *"Hybrid lighting and photovoltaic systems"*, R. D. Costa, **Hiroshima University**, Hiroshima, Japan, December 2018.
33. *"Recent advances in hybrid optoelectronics"*, R. D. Costa, **National Institute for Materials Science (NIMS)**, Tzukuba, Japan, December 2018.

3.8. Awards

1. Career Award, Spanish Society of Materials (SOCIEMAT), July 2018, **J. LLorca.**
2. Best Young Researcher Award, Carlos III University of Madrid, 2018, **J. M. Molina.**
3. Miguel Catalán to scientist in Madrid under 40, Madrid Regional Government, November 2018, **J. J. Vilatela.**
4. XIII Science-Technology award Ciutat d'Algemesí, Ayun. Algemesí, February 2018, **R. D. Costa.**
5. Young Scientist New Champions class 2018 by the World Economic Forum (WEF), September 2018, **R. D. Costa.**
6. Award of the Technical University of Madrid to the best doctoral thesis, 2018, **X. Zhao.**
7. Award of the Technical University of Madrid to the best doctoral thesis, 2018, **L. W. Yang.**

3.9. Seminars

1. *"Emerging materials for electrocatalysis"* **Prof. Jiacheng Wang** (from Chinese Academy of Sciences, CAS). February 2018.
2. *"The quest for new materials: interface-engineered materials"* **Prof. Efstathios I. Melts** (from University of Texas at Arlington). March 2018.
3. *"The challenge of finding critical resolved shear stress values for meso-scale modeling of titanium alloys"* **Dr. Thomas Bieler** (from Michigan State University). April 2018.
4. *"Nanoengineering thermoelectrics to improve their efficiency: some examples"* **Prof. Marisol-Martín González** (from the Institute of Micro and Nanotechnology, at the National Research Center of Spain – IMN-CSIC). April 2018.
5. *"Alloys for additive manufacturing, alloys by additive manufacturing"* **Dr. Eric Jägle** (from Max Planck Institute of Metals Research). May 2018.
6. *"Synergistic CVD graphene and ALD alumina for permeation barrier applications"* **Dr. Indrat Aria** (from Cranfield University). May 2018.
7. *"3D printing technologies, new possibilities for customized products and services for TOC"* **Carlos M. Atienza** (from Biomechanics Institute of Valencia). June 2018
8. *"Engineered electrodes for efficient energy storage and battery safety"* **Dr. Vilas G. Pol** (from Purdue University). July 2018.
9. *"Synchrotron laminography: a technique for in situ observation of damage and its evolution inside engineering materials"* **Dr. Lukas Helfen** (from Karlsruhe Institute of Technology). July 2018.
10. *"Advanced composite materials: manufacturing quality products efficiently"* **Prof. Piaras Kelly** (from University of Auckland). August 2018.
11. *"Microgravity experiments on solidification"* **Dr. Laszlo Sturz** (from Access e.V.). September 2018.

12. *"Discrete slip crystal plasticity modeling of deformation in nanolayered materials"* **Prof. Iromrene J. Beyerlein** (from University of California). October 2018.
13. *"Rational design of carbon nitride materials by supramolecular preorganization of monomers"* **Prof. Jesús Barrio** (from Ben-Gurion University). October 2018.
14. *"New models for description of plastic anisotropy of single crystals and polycrystals"* **Prof. Oana Cazacu** (from the University of Florida). October 2018.

4. Technology offer

The IMDEA Materials Institute is constantly developing new technologies and inventions based on the results of our R&D projects. Here you can find an on-line catalogue gathering the technological offer ready to be transferred to industry, other research insitutions, investors or entrepreneurs.

New Materials Science and Engineering technology which is available for licensing:

Electrode for capacitive deionization

Electrode for capacitive deionization in which the active phase and the current collector are included in a single element, i.e. a composite material.

Opportunity: Technology license

VIPER (VIrtual Ply propERty)

Simulation tool developed by IMDEA Materials to predict ply properties of fiber-reinforced composite materials from the properties and spatial distribution of the different phases and interfaces in the composite.

Opportunity: Software license

FFTMAD (Fast Fourier Transform based homogenization code, MADrid)

FFT-based simulation tool developed by IMDEA Materials for computational homogenization of any heterogeneous material, such as composites, polycrystals or celular materials, by simulating the behavior of a Representative Volume Element of the microstructure.

Opportunity: Software license

Multifunctional sensor for composite materials

Thin sensor laid between dry fabric layers and connected to a simple electrical power meter, that provides real-time information about the resin flow and the gel point during resin infusion and curing, remains embedded in the composite and can be used for structural health monitoring (SHM) and damage detection.

Opportunity: Technology license

MULTIFOAM

Simulation tool developed within the framework of computational micromechanics by IMDEA Materials to predict the mechanical behavior of low to medium density foams with open and closed-cell microstructure

Opportunity: Software license

Resistive curing of polymers and composite materials

Resistive heating of polymer formulations with a very small fraction of conductive nanocarbon materials. Processing of the polymer can be carried out with conventional power supplies, either with AC or DC.

Opportunity: Technology license

MUESLI

MUESLI, a Material UnivErSal LIbrary, is a collection of C++ classes and functions designed to model material behavior at the continuum level. It is available to the material science and computational mechanics community as a suite of standard models and as a platform for developing new ones.

Opportunity: Software license

IRIS

IRIS is an object oriented, general purpose, parallel code for computational mechanics in solid, fluid, and structural applications. It has finite element and meshless capabilities, a wide range of material models, and solvers for linear and nonlinear, stationary and transient simulations.

Opportunity: Software license

CAPSUL

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

Opportunity: Software license

5. Training, communication and outreach

5.1. Theses

PhD Theses

1. *"Synthesis of nano-flame retardant and its use as a promising substitute of antimony trioxide in flame retardant flexible poly(vinyl chloride"*
   Student: Yetang Pan
   Technical University of Madrid (UPM)
   Advisor: Dr. De-Yi Wang
   Date of defense: Februrary 2018

2. *"Computational micromechanics models for damage and fracture of fiber-reinforced polymers"*
   Student: Miguel Herráez
   Technical University of Madrid (UPM)
   Advisor: Prof. Carlos González / Dr. Claudio Saul Lopes
   Date of defense: July 2018

3. *"Multiscale characterization and modelling of polyurethane foams"*
   Student: Mohammad Marvi
   Technical University of Madrid (UPM)
   Advisor: Prof. Javier LLorca / Dr. Claudio Saul Lopes
   Date of defense: July 2018

4. *"Ignition delaying and smoke suppression study of fire-retardant polymer composites"*
   Student: Zhi Li
   Technical University of Madrid (UPM)
   Advisor: Dr. De-Yi Wang
   Date of defense: July 2018

5. *"Development of multifunctional flexible and structural supercapacitors based on CNT fibers"*
   Student: Evgeny Senokos
   Technical University of Madrid (UPM)
   Advisor: Dr. Juan José Vilatela
   Date of defense: September 2018

6. *"Energy harvesting materials based on Carbon nanotubes fiber for tough electronics"*
   Student: Alfonso Monreal
   Technical University of Madrid (UPM)
   Advisor: Dr. Juan José Vilatela
   Date of defense: October 2018

7. *"Numerical methods for the simulation of high velocity impact"*
   Student: Daniel del Pozo Galán
   Technical University of Madrid (UPM)
   Advisor: Prof. Ignacio Romero
   Date of defense: November 2018

Master/Bachelor Theses

1. *"Thin film lighting devices and their electroluminescence features"*
   Student: Jiayin Yu
   Technical University of Madrid (UPM) -Beihang University
   Advisor: Dr. Rubén Costa
   Date of defense: June 2018

2. *"Effect of annealing temperature on the microstructure and mechanical properties of a low carbon steel processed by UFH method"*
   Student: Estela Nario
   Technical University of Madrid (UPM)
   Advisor: Dr. Ilchat Sabirov
   Date of defense: July 2018

3. *"Electrochemical properties of SWCNTs"*
   Student: Beatriz Rodriguez Fernández
   Carlos III University of Madrid (UC3M)
   Advisor: Dr. Juan José Vilatela
   Date of defense: July 2018

4. *"Sensorización y actuación en procesos de fabricación de materiales compuestos"*
   Student: María Fernández Carbayo
   Technical University of Madrid (UPM)
   Advisor: Prof. Carlos González
   Date of defense: July 2018

5. *"Sensores de fibra de nanotubos de carbono para fabricación de material compuesto mediante infusión"*
   Student: Celia Daniela Ramos Cordova
   Technical University of Madrid (UPM)
   Advisor: Prof. Carlos González
   Date of defense: July 2018

6. *"Nuevos materiales de electrodos nanoestructurados para la próxima generación de batería Li-S"*
   Student: Álvaro Muñoz Mauricio
   Carlos III University of Madrid (UC3M)
   Advisor: Dr. Vinodkumar Etacheri
   Date of defense: July 2018

7. *"Preparación y caracterización de materiales compuestos poliméricos resistentes al fuego para aplicación en cubiertas de cables"*
   Student: Ernesto Prudencio Díaz
   National Distance Education University (UNED)
   Advisor: Dr. De-Yi Wang
   Date of defense: July 2018

8. *"Estudio de compuestos estructurales con capacidad de almacenamiento de energía para la electrificación del transporte"*
   Student: Jesús Almenara Rescalvo
   Carlos III University of Madrid (UC3M)
   Advisor: Dr. Juan José Vilatela
   Date of defense: September 2018

9. *"Stretchability and piezoresistivity of Carbon nanotube fibers and their application as strain sensors"*
   Student: Rodrigo Cárdenas
   UIA
   Advisor: Dr. Juan José Vilatela
   Date of defense: September 2018

10. *"Modeling of thermal conductivity by Fast Fourier Transforms"*
    Student: Gonzalo Álvarez Morales
    Technical University of Madrid (UPM)
    Advisor: Dr. Javier Segurado
    Date of defense: September 2018

11. *"Design and validation of a racing car monocoque made of composite material"*
    Student: Jorge de Iscar Gallego
    Carlos III University of Madrid (UC3M)
    Advisor: Dr. Joseba Mugica
    Date of defense: October 2018

12. *"Prediction of composite ply properties through neutral networks"*
    Student: Joshua Maurizio Kiefer
    TuDelf
    Advisor: Dr. Claudio Saul Lopes
    Date of defense: October 2018

13. *"An analysis of the influence of grain size on the strength of FCC polycrystals by means of computational homogenization"*
    Student: R. A. Rubio
    Technical University of Madrid (UPM)
    Advisor: Dr. Sarra Haouala
    Date of defense: November 2018

5.2. Internships / Visiting students

1. *"Carbon nanotube fibre composites"*
   Student: Alexandre Zoetelief Tromp
   Advisor: Dr. Juan José Vilatela
   Visiting student from: University College London
   Period: January 2018- June 2018

2. *"Calibration and optimization of the pressure of the reactive infiltration process"*
   Student: Alejandro Fernández Guerrero
   Advisor: Dr. Srdjan Milenkovic
   Visiting student from: Technical University of Madrid (UPM)
   Period: January 2018 - January 2018

3. *"Fire retardancy of materials"*
   Student: Gizem Kahraman
   Advisor: Dr. De-Yi Wang
   Visiting student from: Yildiz Thecnical University
   Period: February 2018 - April 2018

4. *"An analysis of the influence of grain size on the strength of FCC and HCP polycrystalsby means of computational homogenization"*
   Student: Rafael Rubio
   Advisor: Prof. Javier Llorca
   Visiting student from: Technical University of Madrid (UPM)
   Period: March 2018 - November 2018

5. *"Development of fire-safe electrolytes"*
   Student: Juan Manuel Moreno Naranjo
   Advisor: Dr. Maciej Haranczyk
   Visiting student from: Complutense University of Madrid (UCM)
   Period: March 2018 - June 2018

6. *"Investigation of flame retardancy properties of some polymers"*
   Student: Elif Busra Celebí
   Advisor: Dr. De-Yi Wang
   Visiting student from: Gebze Teknik University
   Period: April 2018 - April 2018

7. *"Modelización del deslizamiento de fronteras de grano"*
   Student: Jiawei Lu
   Advisor: Dr. Teresa Pérez-Prado
   Visiting student from: Southwest Jiaotong University
   Period: May 2018 - July 2018

8. *"Structural composites, manufacturing"*
   Student: André Rittner Pires Correa
   Advisor: Prof. Carlos González
   Visiting student from: FIDAMC
   Period: May 2017 - November 2018

9. *"Design and application of flame retardant in polymers"*
   Student: Haoda Liu
   Advisor: Dr. De-Yi Wang
   Visiting student from: ENSCL
   Period: May 2018 - August 2018

10. *"Fire retardancy of materials"*
    Student: Solen Garel
    Advisor: Dr. De-Yi Wang
    Visiting student from: ENSCL
    Period: May 2018 - July 2018

11. *"Modelización del deslizamiento de fronteras de grano"*
    Student: María Terol Sánchez
    Advisor: Dr. Teresa Pérez-Prado
    Visiting student from: Technical University of Madrid (UPM)
    Period: June 2018 - August 2018

12. *"Modelización del deslizamiento de fronteras de grano"*
    Student: Ricardo Rodríguez
    Advisor: Dr. Teresa Pérez-Prado
    Visiting student from: Technical University of Madrid (UPM)
    Period: June 2018 - August 2018

13. *"Microstructural characterization of infiltrated samples within EQUINOX project"*
Student: Jonathan Israel Espinoza Correa
Advisor: Dr. Federico Sket
Visiting student from: Complutense University of Madrid (UCM)
Period: June 2018 - September 2018

14. *"Mechanical behavior of triplex steels"*
Student: Rocío Pereyra Gómez
Advisor: Dr. Ilchat Sabirov
Visiting student from: Technical University of Madrid (UPM)
Period: June 2018 - August 2018

15. *"Novel Electrode materials for Al-ion batteries"*
Student: Gent Ferati
Advisor: Dr. Vinodkumar Etacheri
Visiting student from: Washington State University
Period: June 2018 - August 2018

16. *"Fire retardancy of materials"*
Student: Alexandre Fétiveau
Advisor: Dr. De-Yi Wang
Visiting student from: Ecole Polytechnique de l'Université de Nantes
Period: June 2018 - August 2018

17. *"Mechanical properties of battery electrodes"*
Student: Francisco Javier Iváñez Castellano
Advisor: Dr. Jon Molina
Visiting student from: University of Alicante
Period: June 2018 - September 2018

18. *"Systematic identification of constitutive parameters for crystal plasticity models of non-cubic metal alloys"*
Student: Zhuowen Zhao
Advisor: Dr. Teresa Pérez-Prado
Visiting student from: Michigan State Unviersity
Period: July 2018 - August 2018

19. *"Multiscale characterization of advanced materials"*
Student: Óscar Nieto Cordero
Advisor: Dr. Federico Sket
Visiting student from: Technical University of Madrid (UPM)
Period: July 2018 - September 2018

20. *"Systematic identification of constitutive parameters for crystal plasticity models of non-cubic metal alloys "*
Student: Zhuowen Zhao
Advisor: Dr. Jon Molina
Visiting student from: Univiversity of Michigan
Period: July 2018 - July 2018

21. *"Smart, foldable and multifunctional 2-Dimensional systems"*
Student: Mauricio Terrones Maldonado
Advisor: Dr. Juan José Vilatela
Visiting student from: University Sussex
Period: August 2017 - August 2018

22. *"Fire retardancy of materials"*
Student: Rebecca Harris
Advisor: Dr. De-Yi Wang
Visiting student from: The Intern Group
Period: August 2018 - October 2018

23. *"Thermoforming prepreg chracterisation"*
Student: Koen Van Dam
Advisor: Prof. Carlos Gonzalez
Visiting student from: Eindhoven University of Technology
Period: September 2018 - December 2018

24. *"Design and development of high performance fire-retardant polymers and nanocomposites"*
Student: Andrés Arribas Domingo
Advisor: Dr. De-Yi Wang
Visiting student from: Complutense University of Madrid (UCM)
Period: October 2018 - October 2018

25. *"Synergistic effect between phosphorus–silicon materials and intumescent flame retardants"*
Student: Juan Li
Advisor: Dr. De-Yi Wang
Visiting student from: Zhejiang University
Period: October 2017 - February 2018

26. *"Simulation of the cyclic behavior of Magnesium alloys"*
Student: Mohammad Jalili
Advisor: Dr. Javier Segurado
Visiting student from: Kashan University
Period: December 2018 - December 2018

5.3. Teaching in Masters

1. *"Advanced composite materials"*
Master in Materials Science and Engineering
Carlos III University of Madrid (UC3M)
Professor: Dr. Jon Molina and Dr. Claudio Lopes

2. *"Simulation techniques of materials"*
Master en Ingenieria de Materiales
Carlos III University of Madrid (UC3M)
Professor: Dr. Jon Molina

3. *"Nanomaterials"*
Master in Materials Science and Engineering
Carlos III University of Madrid (UC3M)
Professor: Dr. Juan Jose Vilatela

4. *"Thermal and thermomechanical testing of materials"*
Master in Materials Science and Engineering
Carlos III University of Madrid (UC3M)
Professor: Dr. Srdjan Milenkovic

5. *"Advanced simulation methods"*
Master of Science in Mechanical Engineering
Technical University of Madrid (UPM)
Professor: Prof. Ignacio Romero

6. *"Module L: scientific programming* language: Python"
International Master in Theoretical and Practical Application of Finite Element Method and CAE Simulation
National Distance Education University (UNED)
Professor: Dr. Javier Segurado

7. *"Advanced numerical methods"*
Master in Materials Engineering
Technical University of Madrid (UPM)
Professor: Dr. Javier Segurado

8. *"Modelling and simulation in materials* science and engineering"
Master in Materials Engineering
Technical University of Madrid (UPM)
Professor: Prof. Javier Llorca, Prof. Carlos González, Dr. Javier Segurado, Dr. Claudio Lopes and Dr. Damien Tourret

9. *"Structural characterization of materials* II: Spectroscopies"
Master in Materials Engineering
Technical University of Madrid (UPM)
Professor: Dr. Federico Sket

10. *"Design and fabrication of advanced* composite materials"
Master in Materials Engineering
Technical University of Madrid (UPM)
Professor: Prof. Carlos González and Dr. Claudio Lopes

11. *"Impact behaviour of materials"*
Master in Materials Engineering
Technical University of Madrid (UPM)
Professor: Dr. Claudio Lopes

12. *"Nanocomposites"*
Master in Materials Engineering
Technical University of Madrid (UPM)
Professor: Dr. De-Yi Wang

13. *"Polymeric materials for advanced* applications"
Master en Ingenieria de Materiales
Technical University of Madrid (UPM)
Professor: Dr. De-Yi Wang

14. *"Non conventional composite materials"*
Master in Composite Materials
Technical University of Madrid (UPM)/ AIRBUS
Professor: Prof. Javier Llorca

15. *"Advanced composites"*
Master in Composite Materials
Technical University of Madrid (UPM)/ AIRBUS
Professor: Dr. Juan Jose Vilatela

16. *"Metal matrix composites"*
Master in Composite Materials
Technical University of Madrid (UPM)/ AIRBUS
Professor: Dr. Ilchat Sabirov

17. *"Numerical simulation techniques"*
Master in Composite Materials
Technical University of Madrid (UPM)/ AIRBUS
Professor: Prof. Carlos Gonzalez, Dr. Claudio Lopes and Dr. Javier Segurado

18. *"New metallic materials for additive* manufacturing"
Master in Additive Manufacturing and Engineering
EDDM Training, Madrid
Professor: Dr. Teresa Perez-Prado

19. *"Science and engineering: advanced* spectroscopic techniques"
Master in Advanced Science and Engineering Materials
Waseda University
Professor: Dr. Ruben Costa

20. *"Science and engineering: solid-state* optoelectronics"
Master in Advanced Science and Engineering Materials
Waseda University
Professor: Dr. Ruben Costa

5.4. 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 European Composites, Plastics and Polymer Processing Platform (ECP4)*
5. *Local Contact Point of the EURAXESS pan-European initiative*
6. *Technical Secretariat of the Spanish Technological Platform of Advanced Materials and Nanomaterials (MATERPLAT)*
7. *Member of the Spanish Aerospace Platform (PAE)*
8. *Member of the Spanish Technological Platform for Advanced Manufacturing (MANUKET)*
9. *Member of the Madrid Aerospace Cluster (MAC)*
10. *Member of the Network of Research Laboratories of Comunidad de Madrid (REDLAB)*

5.5. Individual participation in committees and other institutions

1. *Member of the Steering Committee of the Spanish Society for Numerical Methods in Engineering (SEMNI). Prof. Ignacio Romero*
2. *Member of the Board of Directors of the Society of Engineering Science. Prof. Javier LLorca*
3. *Honorary Adjunct Professor, Beiing University of Chemical Technology. Dr. De-Yi Wang*
4. *Fellow of Royal Society of Chemistry. Dr. De-Yi Wang*
5. *Member of Beam Time Allocation Panel for nano-imaging and nano-analysis at the ESRF (European Synchrotron Radiation Facility). Dr. Federico Sket*
6. *Member of the Advisory Board of the Spanish Association of Composite Materials (AEMAC). Prof. Carlos González*
7. *Member of the Board of Directors of the Spanish Materials Society (SOCIEMAT). Dr. Teresa Pérez-Prado*
8. *Chair, European Mechanics of Materials Conference Committee. Prof. Javier LLorca*
9. *Council Member of the International Association for Computational Mechanics (IACM). Prof. Ignacio Romero*
10. *Member of the External Advisory Panel of the Institute of Materials (Georgia Tech). Prof. Javier LLorca*
11. *Member of the Academic Advisory Committee for the undergraduate Physics Engineering Degree at Universidad Iberoamericana (UIA), Mexico. Dr. Juan José Vilatela*
12. *Manager, Structural Materials Programme, Spanish National Science Foundation, since 2018. Dr. Teresa Pérez-Prado*

13. *Jury member of the European MIT Innovator Awards 2018 and 2019. Dr. Rubén Costa*

14. *Director of the Spain-China Joint Research Centre of Advanced Materials (JRCAM). Dr. De-Yi Wang*

15. *Member of the International Scientific Committee, IRT Jules Verne, Nantes, France. Dr. Teresa Pérez-Prado*

16. *Member of the International Scientific Committee, NOMATEN Center of Excellence, Zwierk, Poland. Dr. Teresa Pérez-Prado*

17. *Honorary Adjunct Professor, Beiing University of Chemical Technology. Prof. Ignacio Romero*

18. *Guest Professor, Central South University, China. Prof. Javier LLorca*

19. *External Scientific Member ("IPF Fellow") of Leibniz Institute of Polymer Research Dresden, Germany, Dr. De-Yi Wang*

20. *Academic Consultant of United Nation Industrial Development Organization (UNIDO). Dr. De-Yi Wang*

5.6. Outreach

1. *Speaker in the World Economic Forum (WEF) 2018 meeting. September 2018. Rubén Costa*

2. *Participation in the "International Day of Women and Girls in Science" (Roundtable of women scientists and primary and secondary school students, talks at primary/secondary schools and guided visit to IMDEA Materials Institute) promoted by Fundación Madri+d, February 2018. Teresa Pérez-Prado, Andrea Fernández, Elisa Fresta, Vanesa Martínez, María Vila and Clara Galera*

3. *Participation in the institutional video for the STEM plan, Madrid Regional Government, Fundación Madri+d, September 2018. Teresa Pérez-Prado*

4. *Participation in the X Conference of Spanish Space Students, ETSI Aeronáutica, Technical University of Madrid (UPM), November 2018. Talk: "Nuevos materiales para impresión 3D de metales". Teresa Pérez-Prado*

5. *Innovators Under 35 - MIT promotional videos (Video 1, Video 2). Rubén Costa*

6. *Lecturer at II Jornada de Química para Profesores de Instituto organizada por la UV/UPV/UA. April 2018. Rubén Costa*

7. *Participation in the "Science Week Madrid 2018", promoted by Fundación Madri+d. September 2018. Anastasiia Mikhalchan, María Azzurra, Mario Rueda and Xiaolin Qi)*

8. *Participation in the "European Researchers' night Madrid 2018", promoted by Fundación Madri+d September 2018. Mario Rueda and Xiaolin Qi*

9. *Primary school workshop: "Experimentos en clase para entender los materiales". C.P. Príncipe de Asturias, Madrid. May 2018. Miguel Ángel Rodiel*

10. *Collaboration with Formula Student UC3M team, 2018.*

11. *Organisation of primary-secondary school and bachelor-master students visits to IMDEA Materials Institute, 8 visits during 2018 (over 200 students)*

5.7. IMDEA Materials in the media

1. *I+D para lograr edificios más sostenibles,* Teresa Pérez-Prado. In El Mundo newspaper, Suplemento Infraestructuras, 22 February 2018.
2. *Better Dye-Sensitized Solar Cells.* Rubén Costa. In ChemistryViews, 19 February 2018.
3. *Large surface area lends superpowers to ultra-porous materials.* De-Yi Wang. In Horizon-Magazine.eu, 25 April 2018.
4. *Estabilización de Proteínas para Concentradores Solares Luminiscentes - Beca Leonardo a investigadores y creadores culturales, Fundación BBVA.* Rubén Costa. Media: El Mundo, El Confidencial, Red Leonardo. October 2018.
5. *Interview to Javier LLorca - "La pasión por abordar nuevos retos y cruzar nuevas fronteras es el signo claro de la vocación investigadora".* In Notiweb, Madri+d, 3 September 2018.
6. *Arena que produce luz blanca similar a la del sol. Rubén Costa. Media:* Europapress, Agenciasinc, La Razón, El Mundo Financiero, Notiweb-Madri+d, 20Minutos, Smart-lighting, Quo, ABC, Cuentamealgobueno, Factornoticia, Ladobe, Costacomunicaciones, Lacronicavirtual, Innovadores, Diarioinformación, Rioja2, Madridpress, Elciudadano, Lateuradio, Noticias4espana, Montevideo, Nmas1, Noticias de la Ciencia, MadridPress, Eenewseurope, Novaciencia, Led-profesional, Energías-renovables, El Universal. October 2018.
7. *La Otra Ciencia. Javier LLorca, premio a la mejor carrera científica de la Sociedad Española de Materiales.* In Telemadrid TV, 29 December, 2018.
8. *El 'padre' del BioLED: el español que puede hacer que tu factura de la luz sea más barata y ecológica.* Rubén Costa. In El Mundo newspaper, 23 October 2018.
9. *A hombros de gigantes - Proteínas luminiscentes para las bombillas del futuro.* Rubén Costa. In RTVE, 17 September 2018.
10. *Feature in an article about foreign researchers in Madrid,* Juan José Vilatela. in El Pais newspaper, 5 December 2018.
11. *Las proteínas luminiscentes como las de las medusas podrán sustituir al sistema LED.* Rubén Costa. In Ondacero.
12. *Your home could be lit by jellyfish in the future, World Economic Forum (WEF).* Rubén Costa. Media: Europapress, La Vanguardia, Weforum, Bigthink, Express, Sdpnoticias, Innovadores, Radio Cable, Faro de Vigo, Levante, La Opinión Coruna. November 2018.
13. *Un investigador español, pretende revolucionar el mundo de la iluminación con sus luces más sostenibles y ecológicas.* Ruben Costa, In Telediario TVE, 3 November 2018.
14. *La Otra Ciencia: baterías.* In Telemadrid TV, 29 December 2018.

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