annual report

2020

www.materials.imdea.org

imdea **materials** institute

institute imdea materials

Ignacio Romero
Director, IMDEA Materials Institute
April 2021

annual report
2020
www.materials.imdea.org

words from the director...

This report describes the activities of our Institute in 2020. Hard facts and ratios draw a picture of a scientific institution running at full speed, producing top-quality science and collaborating with industry as well as other research centres.

But this picture is incomplete. The year has been rough for everyone, and for the Institute as well. The global pandemic that has upset everyone and everywhere has, of course, impacted our activities in a great deal, possibly more than what the figures convey.

Our facilities were completely closed for three whole months and later we slowly returned to something similar to our former routine. Soon we were fully functioning, needless to say, adapting our habits to remote working, social distancing, etc. But personal lives have been touched and, although we have not lost any employee to COVID-19, the pandemic has hit our families, close friends, and relatives.

Employees of IMDEA Materials have made great efforts in 2020 to remain productive and engaged. From my privileged position, I have witnessed this attitude from every group at the Institute: research assistants, associates, tenured and non-tenured researchers, technicians, administration and management. This year we have skipped all of our traditional social events, some of which make IMDEA Materials such a special place, but the Institute is now a mature institution and it has responded to this unusual situation as any Director could have wished.

Despite the difficult situation, this year our scientific production has been very good, and our impact has not ceased to grow. We have participated in 59 research projects and collaborated with 32 companies. Looking ahead, we know that upcoming years will bring new challenges, but is reassuring to see that Europe is decided to push research and development to new heights. New opportunities will open for us and we remain optimistic. Partners and stakeholders should be aware that they can still find in our Institute an excellent centre to face whatever will come.

In summary, the Institute has suffered the impact of COVID-19 in 2020, but it has shown surprising strength and toughness. And those are two traits that we, materials scientists, love.

annual report

2020

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editor

IMDEA Materials Institute

graphic design

base 12 diseño y comunicación

D.L.

M-12729-2021

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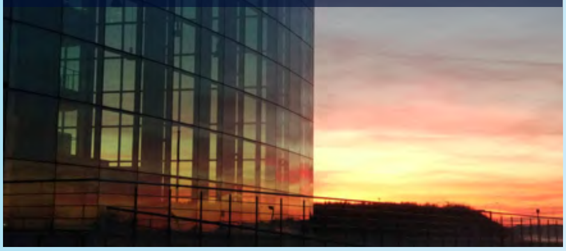
about us



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

IMDEA Materials Institute, one of 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 Materials 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 Materials 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 materials 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

SECTORS AND AREAS OF APPLICATION

RESEARCH PROGRAMMES

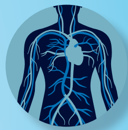

Advanced Materials for Multifunctional Applications


The Next Generation of Composite Materials


Novel Alloy Design, Processing and Development


Multiscale Characterisation of Materials and Processes


Integrated Computational Materials Engineering


Materials for Health Care

The core strength of the Institute is its international research team, consisting of talented researchers from 23 different nationalities, which carries out new scientific discoveries in Materials Science, and fosters the development of emerging technologies.

100 researchers, 23 nationalities,
39% PhDs, 57% foreign researchers
16 research groups

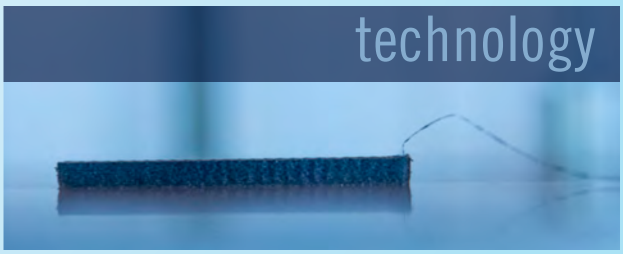
The facilities of IMDEA Materials Institute
The building and laboratories of IMDEA Materials Institute are located at the Scientific and Technological Park of the Technical University of Madrid in Tecnogetafe, Madrid.

2.640 m^2 of research labs

Auditorium (200 people) and networking space for international Conferences and Workshops.

Metals, composites, polymers, 3D printing, multiscale modelling and AI, nanostructured materials, multiscale characterisation of materials and processes, fire resistance and electrochemistry.

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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California Institute of Technology. USA

in figures

human resources

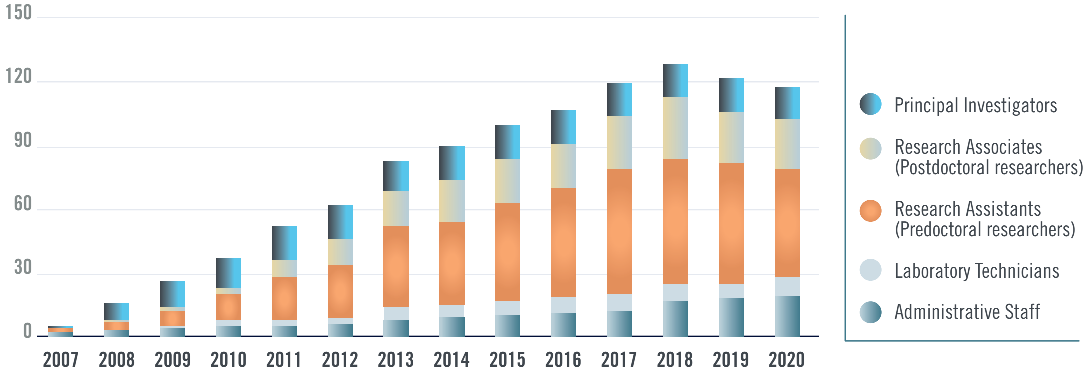
talent

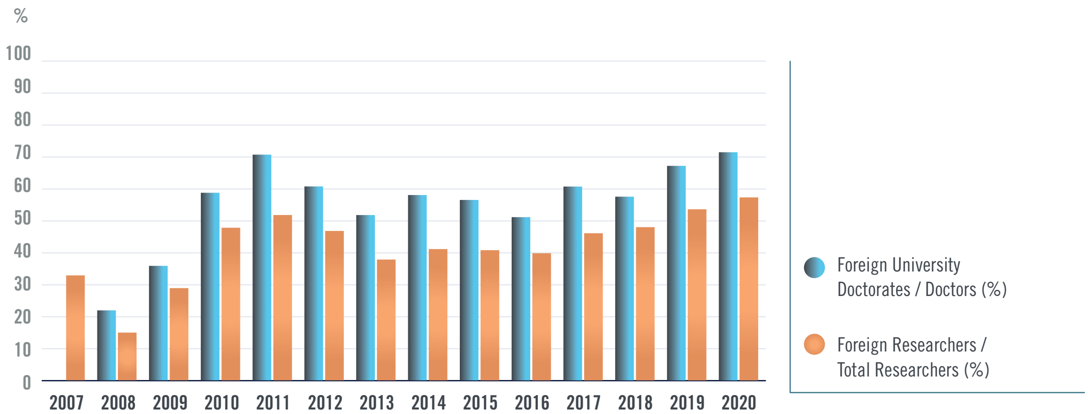
Talent attraction has been the key to the Institute´s **success**.

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**

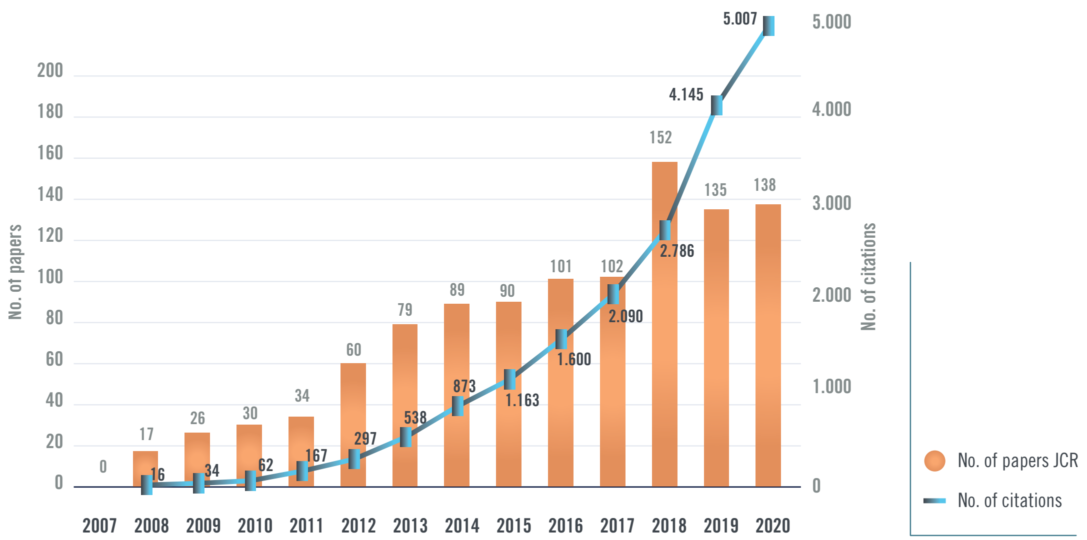
67 defended PhD theses since 2007

56 ongoing PhD theses

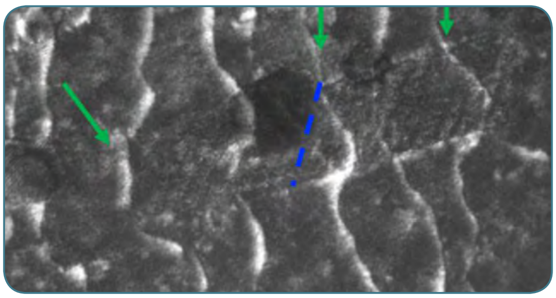
scientific results

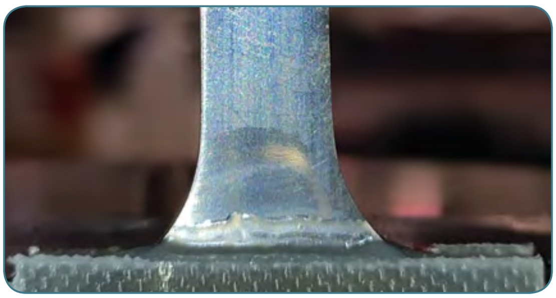
science

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



2020





8 keynote/ invited talks

138 JCR papers

5007 citations

14 invited seminars and lectures

technology transfer and innovation

transfer

As part of our strategic plan 2020-2024, IMDEA Materials Institute has created a Technology Transfer and Innovation Office (TTIO), with the ultimate goal of fostering the output from our research results in terms of exploitation and commercialisation, maximising the impact of the activities of the Institute on the societal needs.

Companies which had active collaborations with the IMDEA Materials Institute in 2020:

Performance indicators in 2020

21 Bilateral projects with industry

4 Industrial doctorates

1 Industrial post-doctoral fellowship

2 Patent applications

10 Patents in portfolio (granted and under evaluation)

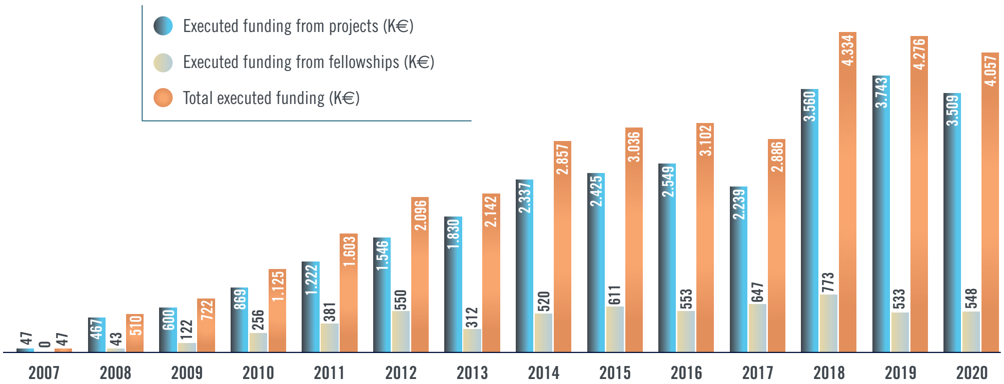
5 Software tools registered (2 licensed)

1 **Valorisation project:** SINERGY - Silicon nanowire fabrics for high energy density batteries (ERC Proof of concept)

erc

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.



2020

International projects 59%

National projects 16%

Regional projects 12%

Contracts with industry 13%

59 R&D projects

2 Active ERC projects

2 Active FET open projects

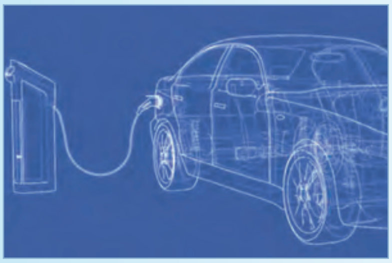
research

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

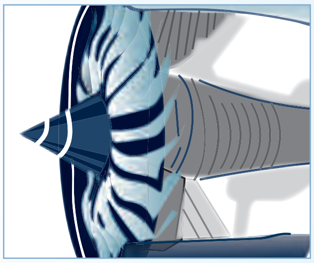


- Synthesis and integration of nanomaterials and polymer-based multifunctional nanocomposites
- New materials and strategies for electrochemical energy storage and conversion
- Computational and data-driven materials discovery

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…)

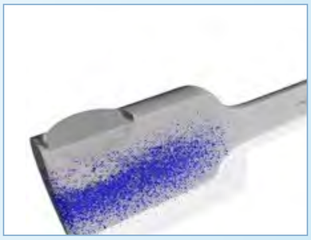
Novel Alloy Design, Processing and Development



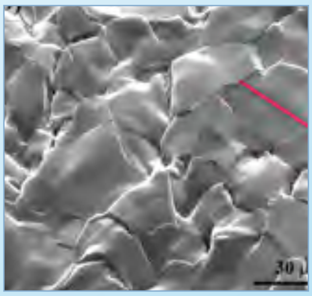
- Structural alloys: light alloys, high temperature alloys and high strength steels
- Characterisation of microstructure and mechanical behaviour
- Advanced manufacturing: solidification and casting, physical simulation of metallurgical processes (rolling, forging, extrusion…)
- Powder metallurgy and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

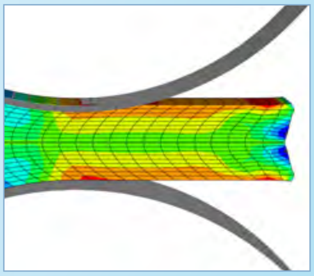


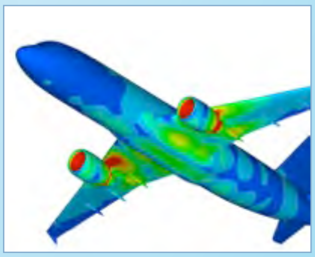
- **4D characterisation:**
  In-situ characterisation of deformation and processes across multiple length scales (750ºC)

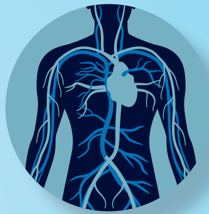


Integrated Computational Materials Engineering

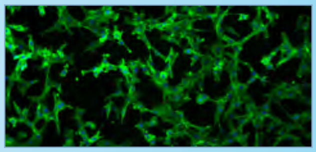
- Virtual materials design, including virtual processing and virtual testing
- Materials modelling at different length and time scales
- Multiscale materials modelling







Materials for Health Care



- Additive manufacturing of biodegradable scaffolds (metallic, polymeric and composites) for tissue engineering (bone, cartilage, skin)
- Biofunctionalization and surface modification on materials with molecules (proteins, peptides, grow factors, drugs) to improve the performance of materials for biological applications and medical devices
- Mechanotransduction: effect of mechanical and electrical stimuli on biological actions
- Manufacturing and application of nanoparticles for drug delivery, disease treatment and antimicrobial activity
- Characterisation of cytocompatibility and biological functionality *in vitro*

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, GLEEBLE 3800 thermo-mechanical simulator equipped with tools for physical simulation of casting, rolling, forging, welding, sintering, and controlled heat treatments.
- Powders manufactured by gas atomisation and mechanical milling. Selective laser melting technology for additive manufacturing of metals.

Polymer based composites and nanocomposites

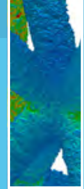
- Liquid moulding processing: RTM resin transfer moulding, VI vacuum infusion, RFI resin film infusion and pultrusion.
- Prepreg lamination using vacuum bagging of autoclave and out-of-autoclave prepregs (OoA) or laminate hot-press moulding (<400°C).
- Semi-industrial equipment for compounding and injection moulding of thermosplastics.
- Integration of advanced nano-fillers.
- Filament maker for 3D printing (3dvo).
- Melt flow index.

Nanomaterials

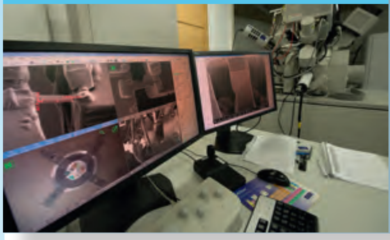
- Synthesis and chemical modification of nanocarbons, inorganic materials, nanoporous semiconductors, thin films, zeolites and other nanomaterials.
- Evaporation equipment in controlled atmospheres, high-pressure reactors and in-house chemical vapour deposition systems.

Energy storage and conversion devices

- Synthesis and characterisation of nanostructured electrode materials for energy storage applications. Fabrication of composite electrodes and integration 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.

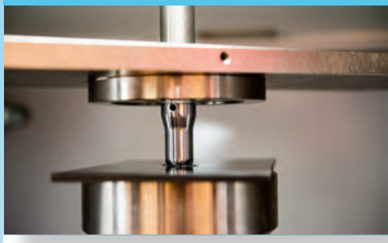


Microstructural and chemical characterisation



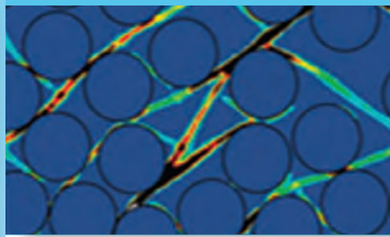
- 3D microscopy at different length-scales, including X-ray tomography, 3D-SEM, 3D-EDS and 3D-EBSD in the FIB and 3D-TEM and 3D-EDS in the TEM.
- In-situ mechanical testing of mininaturised samples in the X-ray tomography system as well as in the SEM and TEM.
- In-situ processing studies in the X-ray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

Mechanical properties



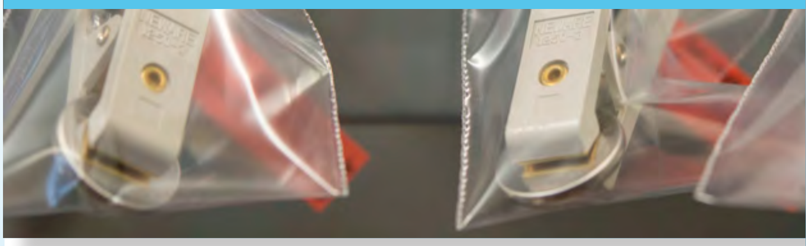
- Mechanical testing of a wide range of materials, using electromechanical and hydraulic machines (quasi-static, dynamic, fracture and fatigue testing in a wide range of temperatures).
- Characterisation of mechanical properties at multiple length scales, including nanoindentation, micropillar compression, 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.

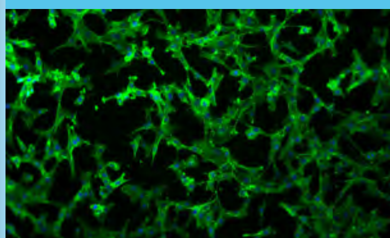
Thermal

- DSC, TGA and Hot Disk Thermal Conductivity analyser. Thermal behaviour of mechanical properties, DMA and rheology.
- 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.
- LCR equipment to quantify dielectric properties in composites.

Cell culture



- Laminar flow hood with aspiration system.
- CO_2 incubator.
- Inverted microscope.
- Centrifuge, water bath, refrigerator and freezer.

programme

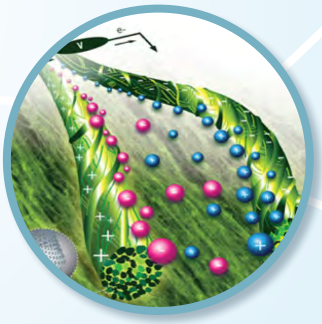
Advanced Materials for Multifunctional Applications

Goal and vision

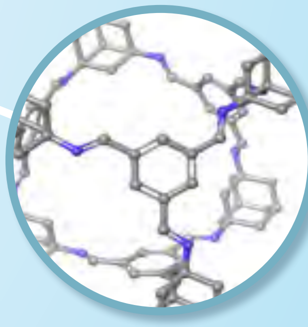
This programme combines expertise in design and synthesis of nano and molecular building blocks with their integration into macroscopic materials and devices. The guiding objective is to simultaneously realise various functions, including fire safety, fire safety energy materials, multifunctional smart materials, high performance and tailored lightweight composites, mechanical properties and efficient energy management, amongst other properties. 33 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



Computational and Data-Driven Materials Discovery

Main research lines

Synthesis and integration of nanomaterials (nanotubes, nanowires, nanofibers and hybrids)

- Synthesis and study of high-performance fibers based on carbon nanotubes.
- Synthesis of nanocarbon/semiconductor hybrids for photo and electrocatalysis, interaction of nanocarbons with liquid molecules, polyelectrolytes and inorganic salts.
- Sensors: chemical, piezoresistive, piezoelectric, triboelectric.
- Hierarchical materials: materials design from the nanoscale to the macroscale, nano-reinforced materials, composite materials with enhanced electrical and thermal conductivity, and fire safety.
- Fire-safe energy materials.
- Phase-change materials for energy storage.

Synthesis and properties of polymer-based multifunctional nanocomposites

- Fire retardant materials via nano-design: multifunctional nanomaterials to increase fire retardancy, e.g. MOF related nanoparticles and lightweight nanocomposites, etc.
- Fire retardant materials via molecular-design: flame retardant polymer electrolytes, novel environment-friendly flame retardants, etc.
- Sustainable materials: biobased supramolecular polymers and bio-based polymers, 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.

Electrochemical energy storage

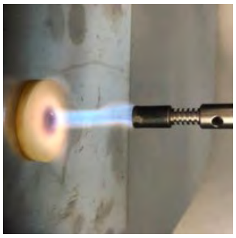
- Tailored designing of nanostructured electrode materials for electrochemical energy storage.
- Engineering of electrode-electrolyte interfaces for high-performance batteries and capacitors
- Spectroscopic and microscopic (in-situ and ex-situ) investigation of ion storage mechanism in energy storage devices.
- Fabrication of flexible battery electrodes for transport and other structural applications.
- Fire safety design and investigation on electrochemical energy storage devices.
- Dry processing of high capacity anodes for Li-ion batteries.
- Synthesis of nanostructured Si anodes for Li-ion batteries.

Computational and data-driven materials discovery

- Discovery of synthetic porous materials for energy-related separations and storage applications (e.g. CO_2 capture, methane and hydrogen storage).
- Design of ionic liquids and polymers.
- Development of modified natural porous materials for selective separation and degradation of organic molecules in food and feed industries.

Concept of CNT fiber as current collectors/active materials for energy management devices.

Defect engineered electrodes.



Fire-safety multifunctional materials.

Projects in focus

SiNERGY / Silicon nanowire fabrics for high energy density batteries

Funding: European Commission/Horizon 2020 Programme – ERC Proof of Concept
Partners: IMDEA Materials Institute
Project period: 2020 - 2022
Principal Investigator: Dr. J. J. Vilatela

Meeting European energy storage in transport, stationary and emerging sectors requires annual cell capacity of at least 200 GWh in the next 5 years, calling for urgent development of new materials for Lithium-Ion Batteries (LIBs) that increase energy/power density at lower costs. Silicon (Si), an abundant material with 10-fold higher capacity than graphite, has shown promise as anode material when appropriately nanostructured. The challenge is in producing nanostructured Si networks using simple and scalable processes leading to thick electrodes that are ultimately economically feasible.

SiNERGY project addresses this challenge by proposing a new simple method for continuous production of nanoengineered self-supported electrodes for high energy density and durable LIBs (see Figure 1), with potential performance nearly an order of magnitude above commercial anodes. Compared to existing processes for Si-anode fabrication, this method eliminates several manufacturing steps, offers feasible scale-up, and unlocks high areal capacity (target 20mAh/g).

The aim of SiNERGY is to conduct R&D activities to:
- Demonstrate LIB performance above commercial technology
- Perform a first analysis of techno-economic scale-up of the manufacturing process to determine operation costs and throughput capacity
- Evaluate their alignment with the LIB market

Figure 1: photograph of a freestanding anode of Si nanowires

Research in focus

Fire retardant battery materials

IMDEA Materials is working on new battery materials that combine electrochemical integrity and enhanced fire safety. Figure 1 below [1] shows a fully solid-state battery based on a HKUST-1 MOF modified electrolyte with simultaneously improved electrochemical performance and fire safety. In Figure 2 [2] a highly flame-retardant phosphazene based gel polymer electrolyte was used to fabricate a lithium-ion battery with simultaneously improved fire retardancy and electrochemical properties. These type of batteries have potential to reduce the huge costs associated to fire accidents in lithium-ion batteries found in electric vehicles, electronics goods, etc.

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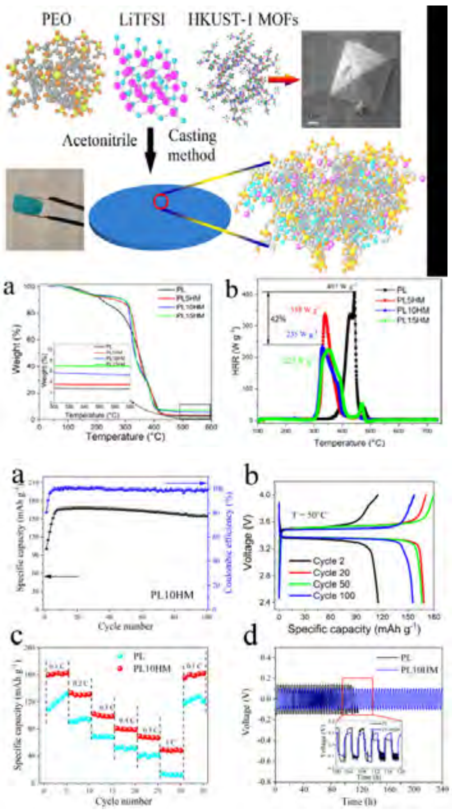

Figure 1: HKUST-1 MOF modified PEO solid-state electrolyte with simultaneously enhanced fire safety (42% reduced peak heat release rate) and electrochemical performance.

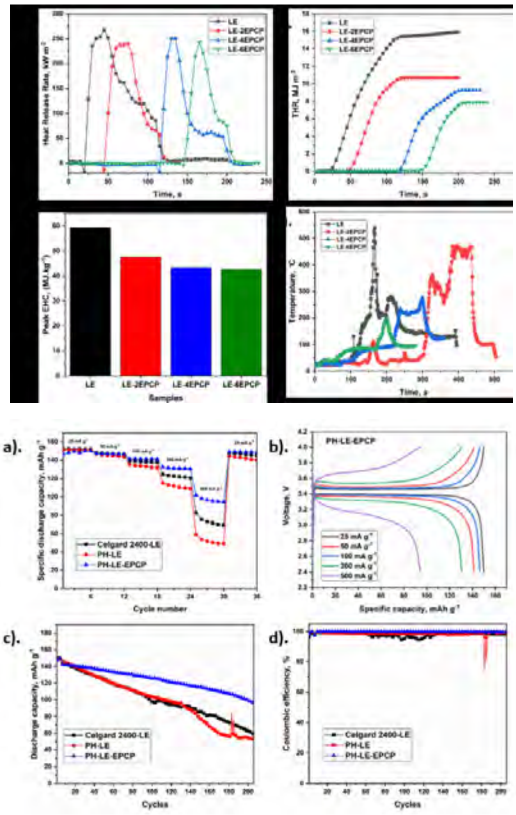

Figure 2: Phosphazene modified PVDF-HFP gel polymer electrolytes with simultaneously enhanced fire safety (>100s of delayed ignition) and electrochemical performance.

[1] A. Yusuf, V. S. Avvaru, M. Dirican, S. Changchun, D-Y Wang, Low heat yielding electrospun phosphenanthrene oxide loaded polyacrylonitrile composite separators for safer high energy density lithium-ion batteries, **Applied Materials Today 20**, *100675 (2020)*
[2] C-C Sun, A. Yusuf, S-W Li, X-L Qi, Y. Ma, D-Y Wang, Metal organic frameworks enabled rational design of multifunctional PEO-based solid polymer electrolytes, **Chemical Engineering Journal 414**, *128702 (2021)*

In-situ studies of defect-engineered electrodes

Diffusion independent pseudocapacitive ion storage is one of the recently investigated mechanisms for achieving ultrafast Li and Na-ion storage. It usually involves surface/ near surface charge-transfer reactions. Nevertheless, intrinsic pseudocapacitance of transition metal oxide anodes is not sufficient to deliver high energy and power densities. Although pseudocapacitance can be induced by nanostructuring and defect/ interface engineering, this method remains elusive in the case of metal oxide anodes. Nanoscale engineering is a potential solution to circumvent the challenges associated with conventional lithium-ion battery electrodes because of their diverse surface properties, tunable structures and improved conductivity. IMDEA Materials has developed defect-engineered (0D, 1D and 2D defects) metal-oxide anodes for high energy/ power density Li/ Na-ion batteries.

Li and Na-ion storage mechanism in most of the pseudocapacitive electrodes reported have not been systematically investigated. Improved performances are often assigned to surface storage, and the exact the mechanism is not clear. Advanced characterization techniques are therefore required to explain the crucial reasons for the defect engineered pseudocapacitive electrodes. For instance, IMDEA Materials has investigated pseudocapacitive Li-ion storage mechanisms (see Figure 1) enabled by nanograin-boundaries of polycrystalline Co_3O_4 nanorods through in-situ X-ray diffraction and Electron Energy Loss Spectroscopy (EELS) analysis. These in-situ measurements can be also employed to investigate the Li/ and Na-ion storage mechanism of a variety of electrode materials.

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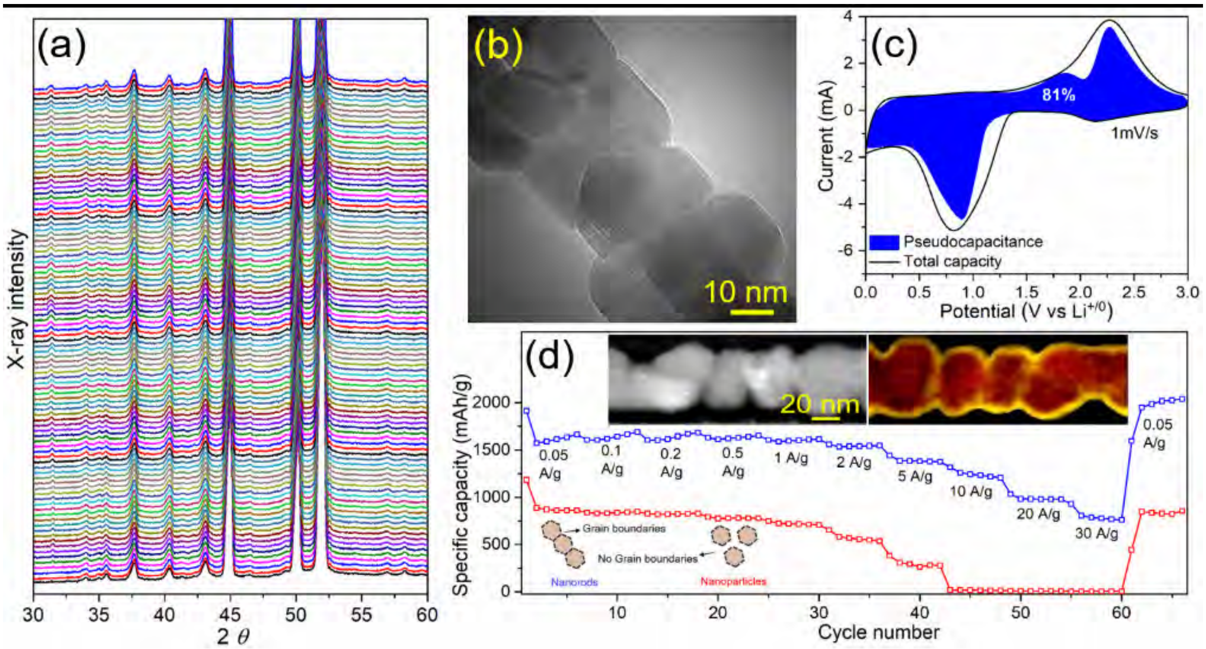


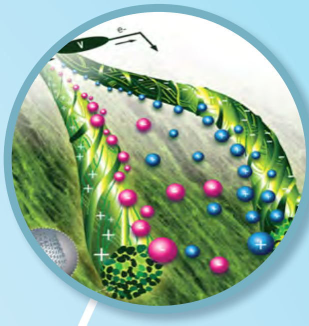
Figure 1: (a) In-situ XRD patterns, (b) HRTEM image, and (c) pseudocapacitive contribution of Co_3O_4 nanorods. (d) Galvanostatic rate performance of Co_3O_4 nanorods and Co_3O_4 nanoparticles at various current densities. Inset: EELS mapping images showing Li (yellow) and Co (red) distribution of Co_3O_4 nanorod electrodes discharged to 0 V.

programme

The Next Generation of Composite Materials

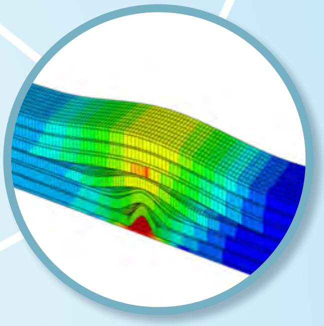
Goal and vision

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 materials science and engineering including manufacturing, optimisation of material performance (damage tolerance and impact resistance), material characterisation at different length scales (nanoindentation, X-ray tomography) and development of modelling tools for both virtual processing and virtual testing. Manufacturing of composites by injection/infusion/pultrusion or prepreg consolidation is assisted by advanced sensors that support the use of smart manufacturing techniques toward process optimisation. Multiscale physically-based simulation tools are envisaged to predict the mechanical performance of structural composites as a function of their structure allowing a significant reduction of costly experimental campaigns.



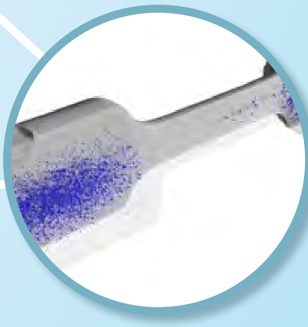
Multifunctional Nanocomposites

High Performance Polymer Nanocomposites



Design & Simulation of Composite Structures

Structural Composites



X-Ray Characterisation of Materials

Nanomechanics

Main research lines

Processing of high performance composites

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

Recycling 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

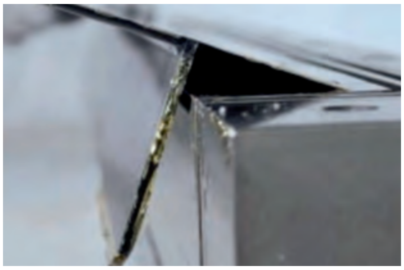
- Multiscale strategies for design and optimisation of composite materials and structures. Behaviour of composite materials and structures under high velocity impact (ice, metallic fragment or blade). Crash-worthiness and failure of composite structures. Effects of defects.

Virtual processing of composites

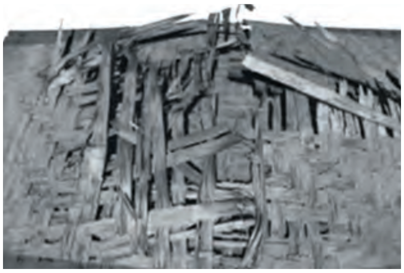
- Manufacturing process simulation. Multiphysics models for manufacturing including forming, injection/infusion process as well as curing. Characterisation of processing parameters.

Digital technologies for structural composites

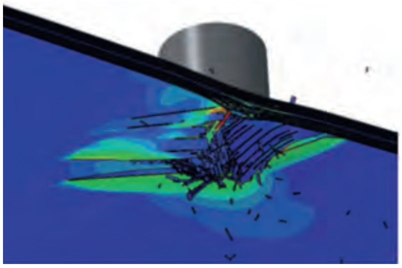
- Methods of artificial intelligence for optimization of composite manufacturing and structural performance. Sensors and process controls. Digital twins and hybrids.



Manufacturing of structural composites.



Multifunctional composites (e.g. lightning impact).



Multiscale virtual testing and processing.

Projects in focus

BINOMIAL/ Evaluation of damage made by ballast impact in composite materials

Funding: Patentes TALGO
Partners: IMDEA Materials Institute
Project period: 2019 - 2020
Principal Investigator: Prof. C. González

Structural composites are being extensively used in those applications driven by lightweight reduction. Among different industries, railway is currently demanding materials to replace aluminum and steel parts enabling efficient weight and cost designs. However, composite materials should pass very stringent conditions in railway such as those related with fire and impact resistance. When railway operates at high-speed, ballast stones from rail infrastructure can be ejected against the rolling stocks producing damages in the form of indentations and delaminations, which can reduce locally the strength of materials.

BINOMIAL project is focused on studying the effect of such impact ballast events on the damage generation in structural carbon composites candidates, monolithic and sandwich, to replace primary structures on the rolling stocks. The project combines experiments and mechanical analysis by numerical simulation. Impacts are performed by replacing the ballast stone with a sharp-tip metallic indentor (see Figures 1 and 2). Damage is subsequently inspected by ultrasounds and X-ray tomography and the residual strength in compression measured (Figure 3). Numerical and analytical models are also used to validate the experimental study.

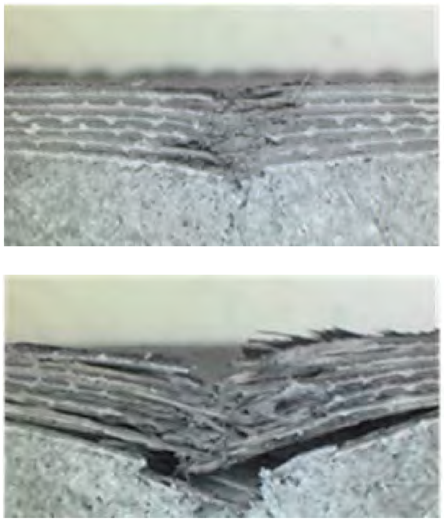


Figure 1. damages induced by simulated ballast impact on the carbon skin of a sandwich laminate for two different impact energy levels.

Figure 2. drop-weight testing frame with the sharp-tip metallic indentor to simulate ballast impact events.

Figure 3. compression after impact strength evaluation.

Research in focus

AI-guided smart manufacturing of structural composites

Manufacturing in the EU is crucial, given that it is one of the main drivers in innovation, job creation and sustainable growth. It involves almost 2,000,000 companies that provide approximately 28.5 million jobs. Therefore, its impact is significant in terms of economic share, with it being ~18% of the EU-27 gross domestic product. However, at present the dependence of processing on external factors or disturbances is still important. With that in mind, the cumulative and recurrent costs for the non-implementation of the appropriate correcting on-the-fly manufacturing policies that could allow recovery from failure will produce, without any doubt, negative impacts on the competitiveness of the EU industrial sector in the future.

IMDEA Materials has developed efficient Artificial Intelligence (AI) methods to automatically detect defects produced during manufacturing of structural composites by liquid moulding by using Virtual Processing (VP) techniques which include [1]:

- Creation of synthetic databases obtained by means of computational mechanics (fluid and solid) for typical manufacturing processes. This includes the use of a comprehensive multiscale and multiphysics VP simulation environment.
- The data generated is used to deliver regression-classification tools for the automated detection of processing disturbances from processing sensor signals.
- Adequate quantification of uncertainty of processing model parameters including model inadequacies.
- A laboratory-scale demonstrator (Figure 1) where the AI tools for automated detection of defects is being deployed. A network of pressure and temperature sensors are distributed on the demonstrator and their corresponding signals used to detect and quantify the presence of a manufacturing disturbance that may produce a defect.

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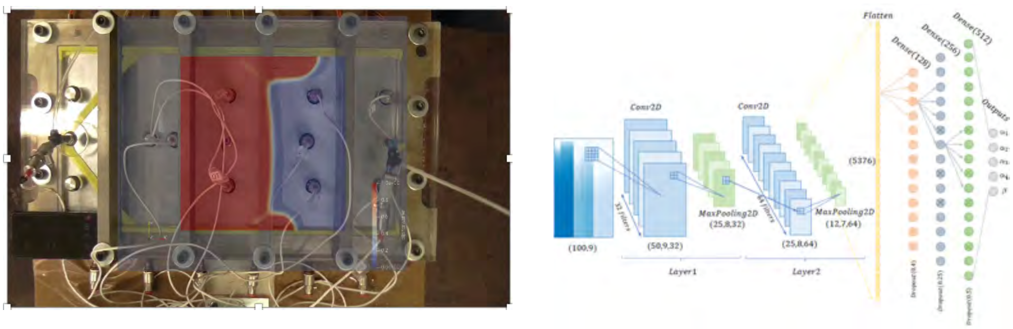

Figure 1: (Left) Laboratory scale demonstrator of injection moulding containing arbitrary race-tracking. The image shows the flow front position (experimental) and the numerical simulation (red). (Right) Deep-learning neural network used to produce regression results from pressure sensor signals.

IMDEA Materials expertise includes the capabilities produce advanced VP modelling of manufacturing process, lab-scale experimental set-up including sensors and actuators, and expertise to develop deep-learning methods.

[1] C. González, J. Fernández-León, A Machine Learning Model to Detect Flow Disturbances during Manufacturing of Composites by Liquid Moulding, **Journal of Composite Science***, 4, 71 (2020)*

3D printing of structural composites by using recycled fibers

Due to the rapid growth in the use of composite materials, environmental concerns have become an increasingly influential topic, making recyclability of composite materials a key issue. Furthermore, several related EU laws have been passed to minimize the environmental impact of composite structures and to make rational use of landfills. However, the number of composites currently recycled is less than 5% of the total amount produced requiring efforts to reuse such kind of waste materials in a circular economy.

IMDEA Materials has developed technologies to manufacture 3D printed composite parts made with recycled fibers obtained from structural composites scraps (Figure 1). The process starts with the recovery of the carbon/glass fibers from cured composite parts or prepreg scraps. It consists of two subsequent steps: a thermolysis or pyrolysis, followed by a gasification or oxidation. In the first one, the separation fibre/resin takes place; in the second stage, the char deposited on the surface of the fibres is removed. After that process, the recovered fiber is subjected to milling to produce short fibers. IMDEA Materials has the possibility to manufacture polymer pellets containing different fiber charges by means of extrusion. These pellets can be used for injection moulding and production of 3D printer filaments (3DEvo) with a variety of diameters and polymers (typically PLA). Filament fused deposition systems as well as advanced short and long fiber 3D printers are available. This capability in combination with expertise in design and optimization of structural composite parts by means of advanced finite element modelling has the potential to be fully exploited in automotive, aerospace and other sectors to produce recycled parts with tailored properties.

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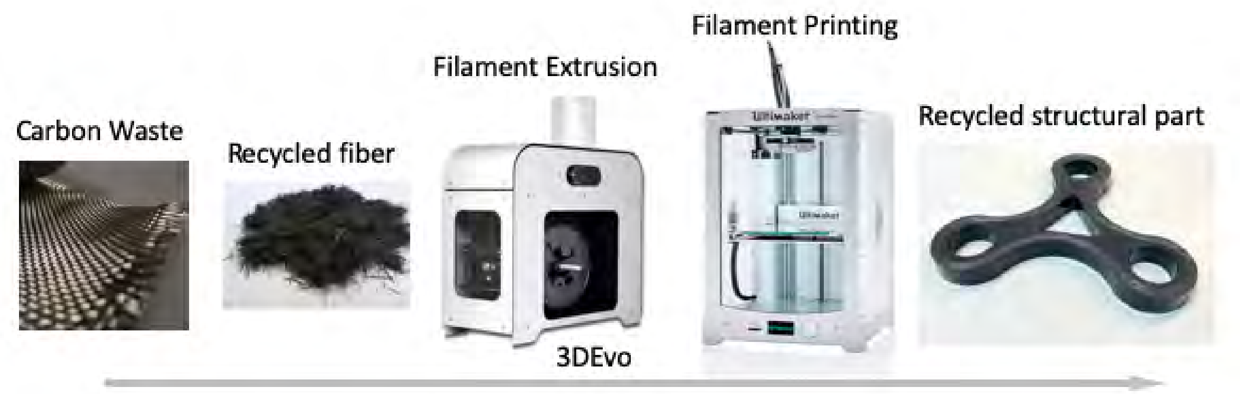
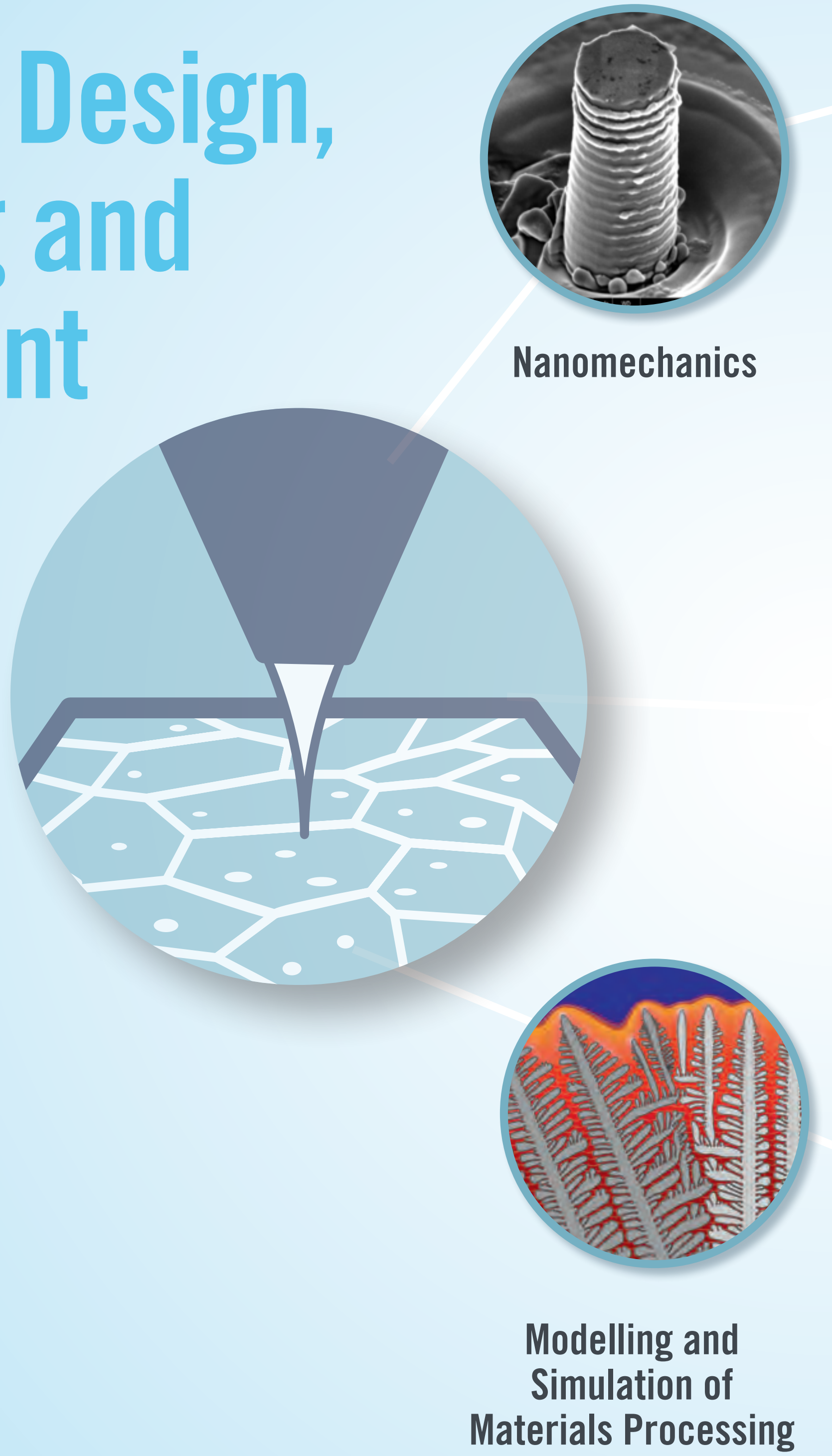


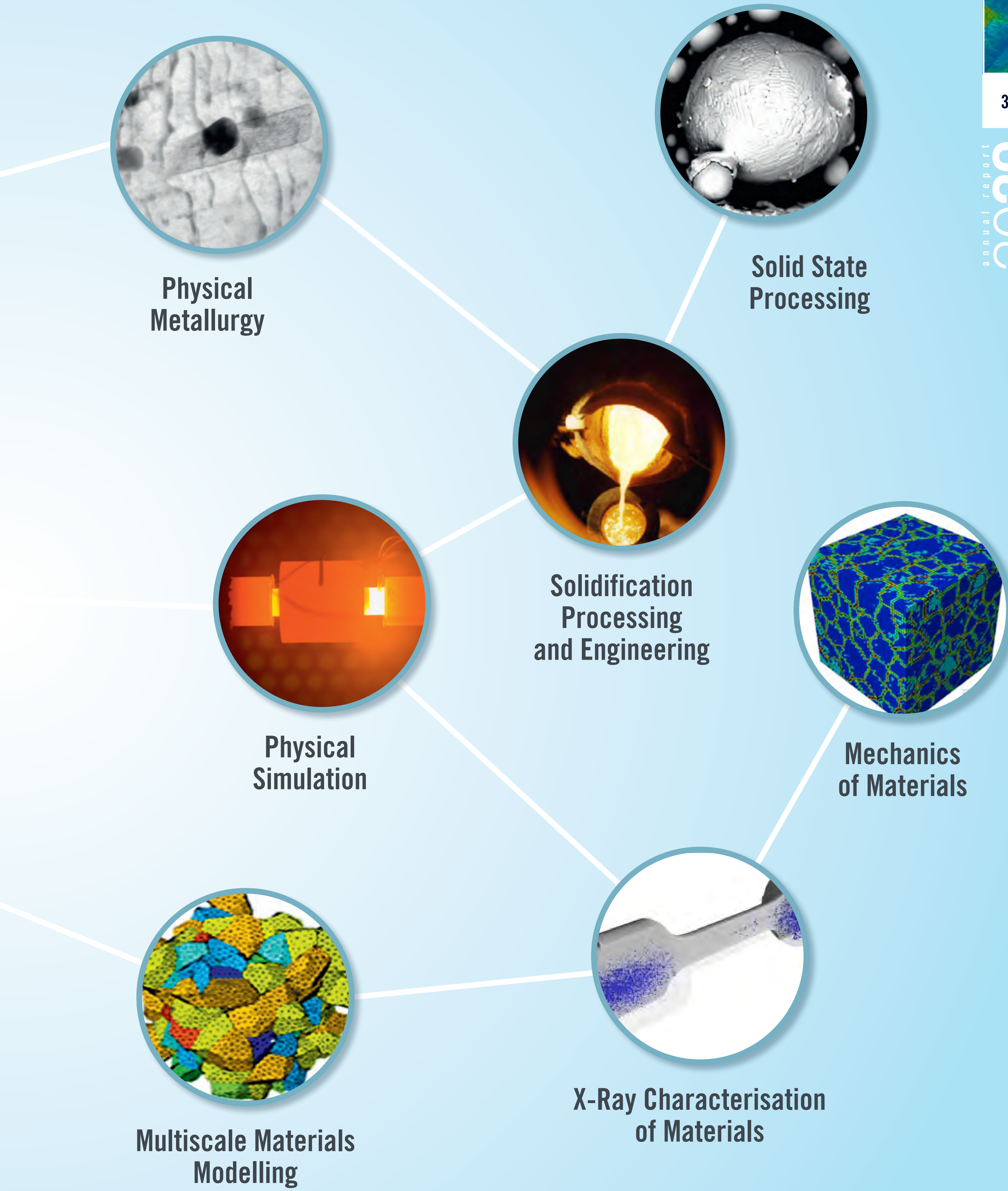
Figure 1: recycling chain from composite waste/scraps to the final recycled structural part.

programme
Novel Alloy Design, Processing and Development



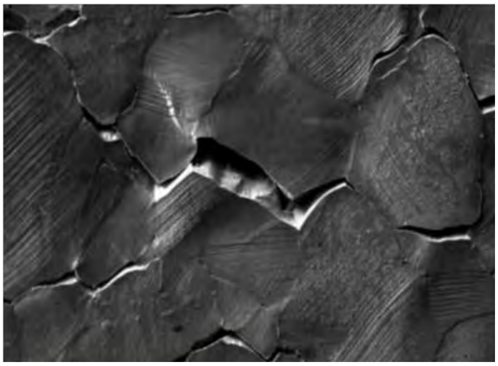
Goal and vision

This 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 laboratory scale (casting, wrought processing, physical simulation of metallurgical processes, atomization, additive manufacturing by selective laser melting, etc), microstructural characterisation (electron microscopy, X-ray diffraction, nanotomography) and mechanical property testing at a wide range of temperatures and strain rates, as well as a range multiscale simulation tools and high-performance computing infrastructure in support of alloy design and process optimisation.

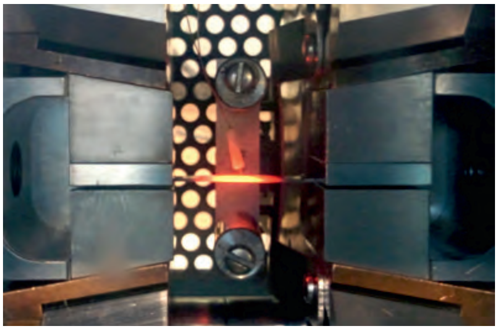

Physical
Metallurgy
Solid State
Processing
Solidification
Processing
and Engineering
Physical
Simulation
Mechanics
of Materials
Multiscale Materials
Modelling
X-Ray Characterisation
of Materials

Main research lines

- **Characterisation** of microstructure and mechanical behaviour.
- **Advanced manufacturing:**
  - Solidification and casting. Centrifugal, suction casting and reactive infiltration.
  - Development of high-throughput methods by physical simulation of metallurgical processes (rolling, forging, extrusion, welding).
- **Powder metallurgy and additive manufacturing:**
  - Powder design, fabrication and characterizing.
  - Process optimization.
- **Virtual processing:**
  Multi-scale modeling of solidification and phase transformations in metallurgical processing of metals and alloys.
- **Virtual testing:**
  Multi-scale modelling of the mechanical behaviour of metallic polycrystals as function of their microstructure.



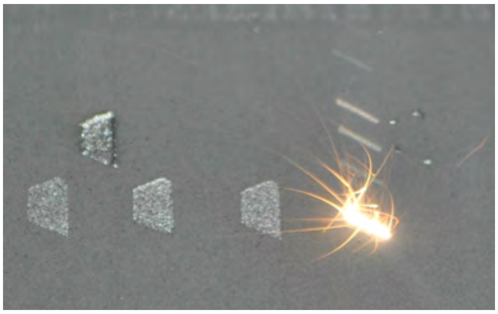
In-situ characterisation.



Thermo-mechanical processes in Gleeble thermo-mechanical simulator.

Materials of Interest

- **Metallic alloys for high temperature structural applications.** Ni/Co-based superalloys, High Entropy Alloys, 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.



Advanced manufacturing.

Projects in focus

DELIGHTED / Design of Lightweight Steels for Industrial Applications

Funding: European Commission/ Research Fund for Coal and Steel (RFCS)
Partners: IMDEA Materials Institute (Coordinator), Ghent University, Ocas NV, Politecnico di Milano, Max Planck Institute for Iron Research
Project period: 2020 - 2023
Principal Investigator: Dr. I. Sabirov

Triggered by environmental issues, the EU market has a strong interest in development of low-cost and lightweight heavy gauge steels for various applications. The austenitic Fe–Al–Mn–C quaternary alloys have recently been attracting tremendous attention, as they can demonstrate exceptional combination of high strength and high ductility, and do not need expensive strategic alloying elements like Mo, Cr and/or Ni, though they are hard to process materials. The aim of the DELIGHTED project is to gain fundamental understanding of principles of microstructural design for engineering of perspective austenitic lightweight steels to reach the combination of mechanical and performance properties suitable for applications (see Figure 1).

The main objectives of the DELIGHTED project are:

- To understand the effect of the steel chemistry on the microstructure evolution during hot rolling including recrystallization, precipitation and growth of particles and development of crystallographic texture.
- To understand fundamentals of cracking during hot rolling of austenitic lightweight steels, which is necessary for development of novel thermo-mechanical processing routes.
- To describe kinetics of kappa-carbide precipitation and growth in the austenitic matrix with respect to the steel chemistry and heat treatment parameters.
- To establish the relationships between microstructural features of lightweight steels and various technological properties, such as fracture toughness, fatigue resistance, weldability, etc.
- To establish the microstructure – properties relationship in the form of analytical models predicting the mechanical properties of lightweight steels.
- To understand the principles of microstructural design for engineering of lightweight steels exhibiting a combination of enhanced performance properties with improved mechanical strength.
- To design and manufacture a prototype of a cabin for vineyard mini-tractor with the connections made of the developed lightweight steel and to experimentally measure its crash resistance.

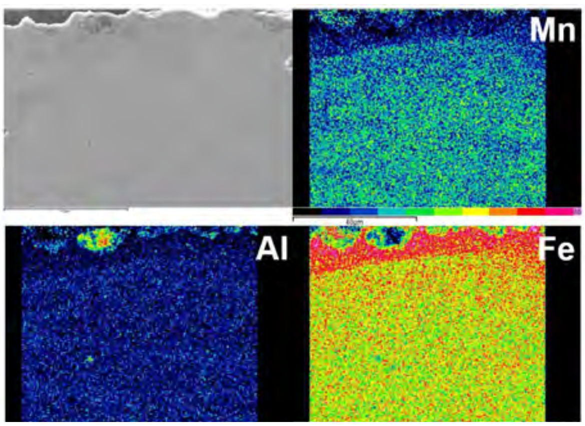


Figure 1: elemental map of the main alloying elements in the subsurface area of a hot rolled Fe-30Mn-9Al-1C steel.

Research in focus

New 3D-printed alloys for extreme conditions

IMDEA Materials has recognized expertise on the design of alloys for high temperature, high strength and lightweight applications, which are suitable for the production of 3D printed components by laser-based or binder-jetting methods. Previous works include the design of superalloys for turbine components, either in solid form or as lattice structures, as well as the definition of tuned compositions for high strength Al alloys with higher hardness than conventional wrought products. IMDEA Materials is also a global leader on the design and optimization of Mg alloys for sustainable transportation and has successfully developed new intermetallics, high performance steels and high entropy alloys. The competitive advantage of IMDEA Materials lies on its deep understanding of the processing-microstructure-mechanical property relationships, that is grounded on solid knowledge on physical metallurgy concepts, as well as on proven experience on microstructure and mechanical property characterization at all length scales.

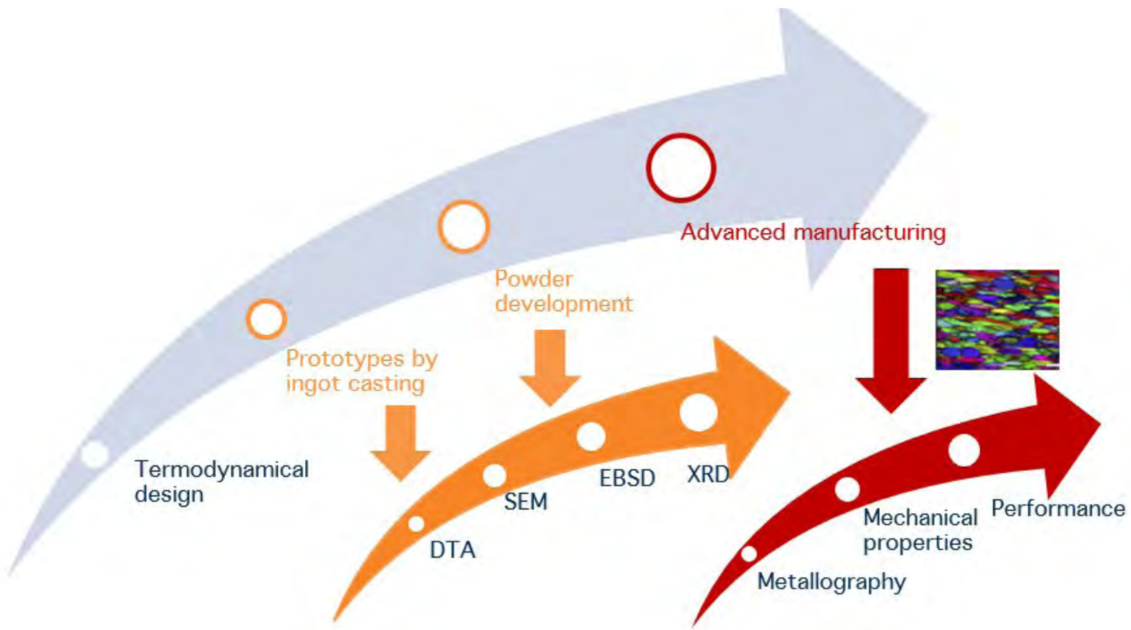
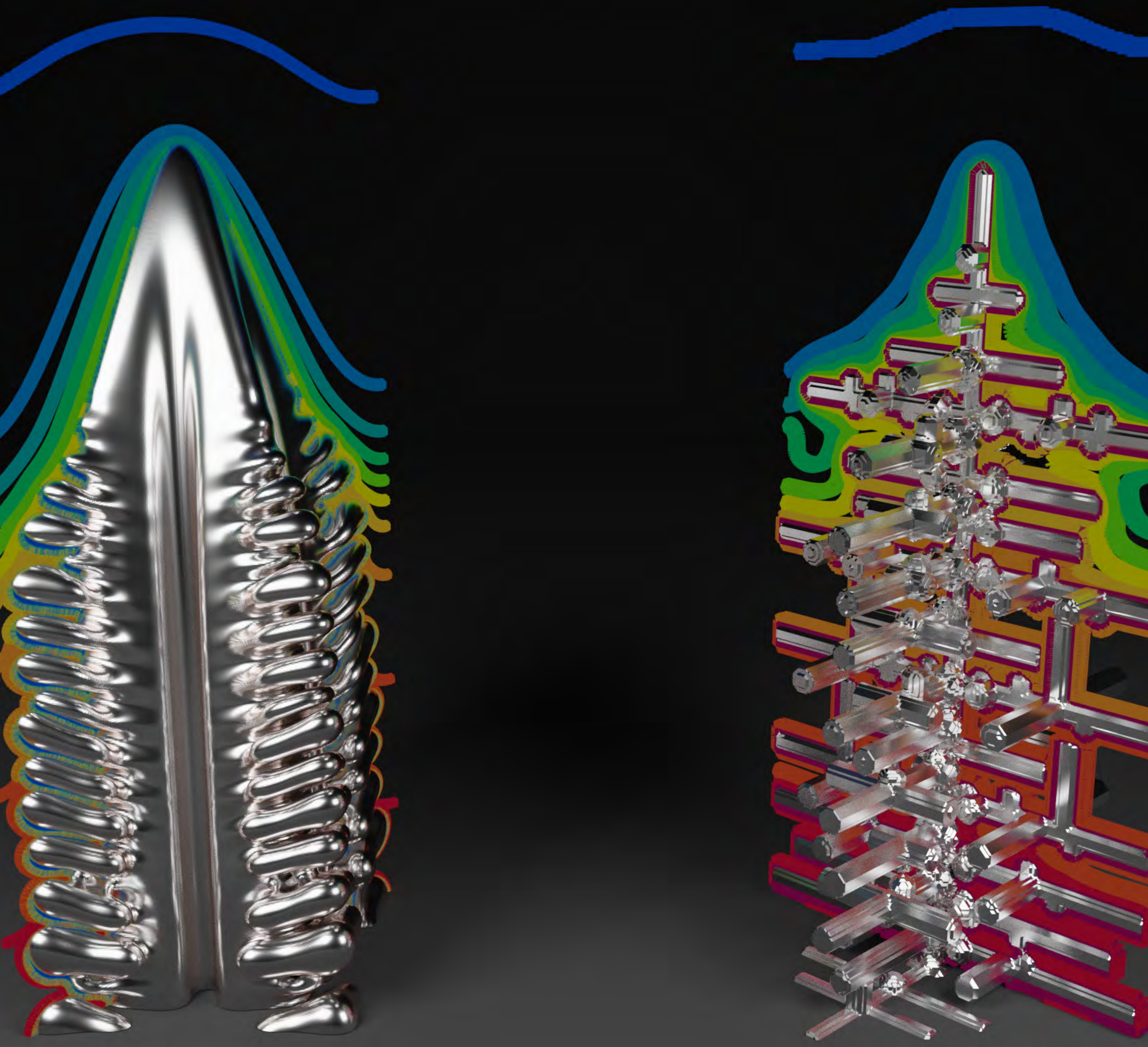


Figure 1: summary of the capabilities available at IMDEA Materials for the development of 3D-printed alloys



Solid-liquid interfaces of Al-Cu dendrites growing from the liquid melt. Winner imaging contest 2021. Simulation

IMDEA Materials has a one-stop shop for the development of 3D-printed alloys. Experimental facilities (Figure 1) include:

- Processing: ARCAST 200 arc melting and casting furnace furnished with laboratory scale gas atomizer.
- 3D printing: AM400 Renishaw selective laser melting 3D printer.
- Powder characterisation: Hall flowmeter, particle size analyzer, sieves.
- Structure characterisation: X-ray diffractometer, FIB-FEGSEM and FEG-S/TEM microscopes.
- Sample preparation, thermal treatments and mechanical testing at all length scales and conditions.

Experimental capabilities are complemented by a suite of simulation tools. Computational models cover a broad range of length/time scales, from the atomic structure of interfaces to the macroscopic scale of entire components. These tools, coupled together and tailored to tackle specific technological challenges. More details about these simulation tools are given in the research in focus entitled "Predictive simulation of metal additive manufacturing. From composition and processing to mechanical properties".

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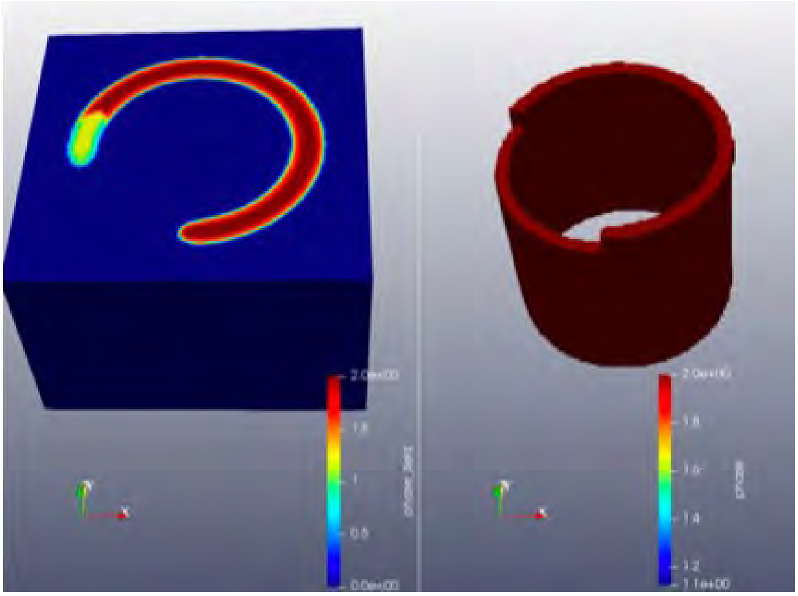

Figure 2: finite element modelling of selective laser melting processing. Temperature (left) and layer-by-layer addition of materials by selective melting (right)

Physical simulation of joining of dissimilar materials

IMDEA Materials has developed a physical simulation tool to predict joinability of dissimilar metallic materials with different melting points. Very small samples of the actual dissimilar materials are subjected to the same thermal and mechanical profiles in a thermo-mechanical simulator (GLEEBLE 3800) that they would experience on a larger scale. Analysis of the processed samples allows to determine the quality of the joint, the microstructure and properties of the newly formed interface, as well as to pick up the optimum processing parameters for joining. This approach allows making faster ‘go / no go’ decisions for joining dissimilar materials, and dramatically reduces the time and cost to develop novel processing routes. This technology has already successfully used for physical simulation of friction melt bonding of a steel and Al alloy (see Fig. 1 and [1]) and can be further optimized for physical simulation of metal/polymer or metal/composite joining.

For more information, please contact
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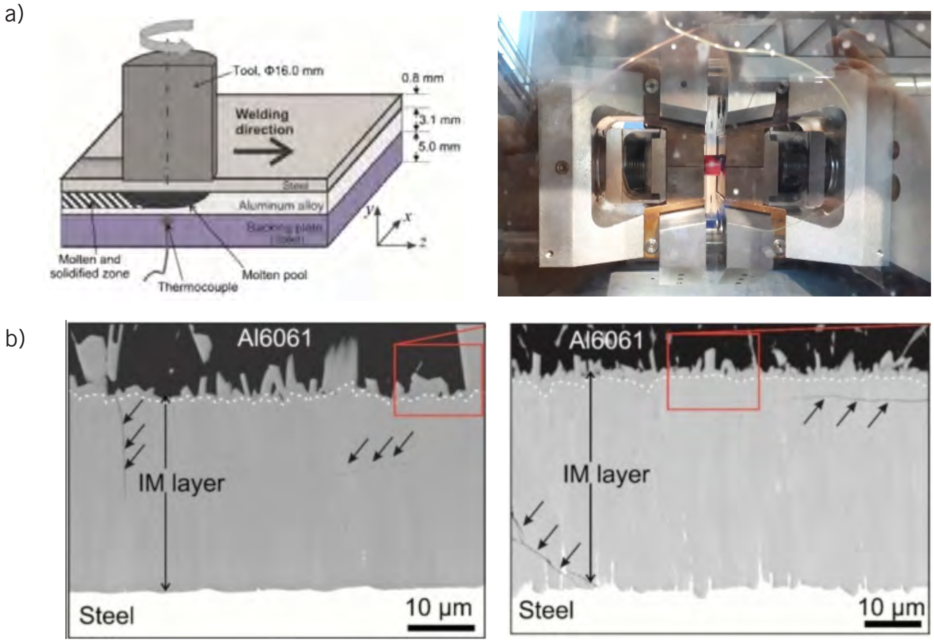


Figure 1: a) Schematic presentation of friction melt bonding (left) and its simulation in GLEEBLE 3800 (right); b) Newly formed interface after friction melt bonding of steel and Al6061 alloy (left) and its prediction via physical simulation (right).

IMDEA Materials has also significant expertise in the multiscale microstructural characterization of joints and interfaces, as well as their mechanical characterization on various scales. This allows studying the link between joining parameters, microstructure of joints and their properties. The understanding of the processing – microstructure – properties relationship enables further optimization of joining processes.

[1] T. Sapanathan, N. Jimenez-Mena, I. Sabirov, M.A. Monclús, J.M. Molina-Aldareguía, P. Xia, L. Zhao, A. Simar. A new physical simulation tool to predict the interface of dissimilar aluminum to steel welds performed by friction melt bonding. **Journal of Materials Science & Technology**, *35 2048-2057 (2019).*

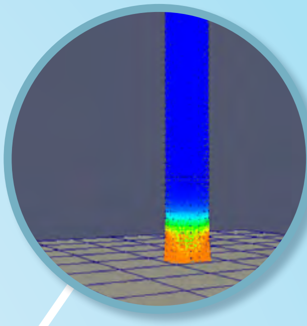
programme

Integrated Computational Materials Engineering

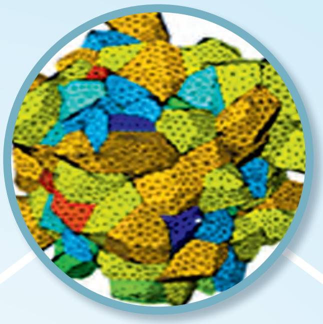
Goal and vision

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.

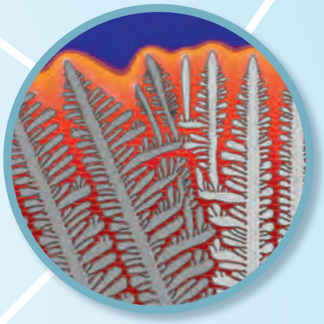
The expertise of the researchers in the programme covers a wide range of simulation techniques at different scales (electronic, atomistic, mesocopic and continuum) and is supported by a high performance computer cluster.



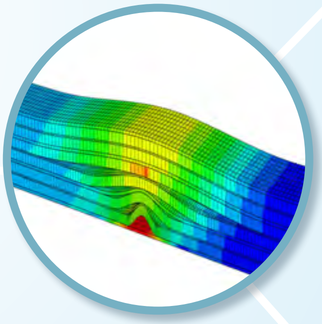
Computational Solid Mechanics



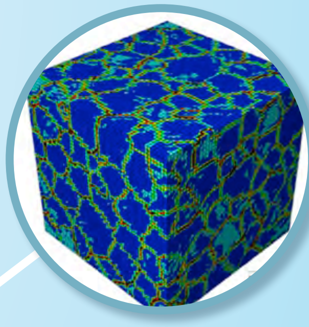
Multiscale Materials Modelling



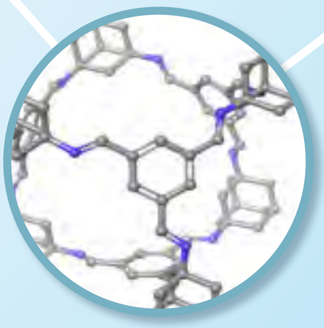
Modelling and Simulation of Materials Processing



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

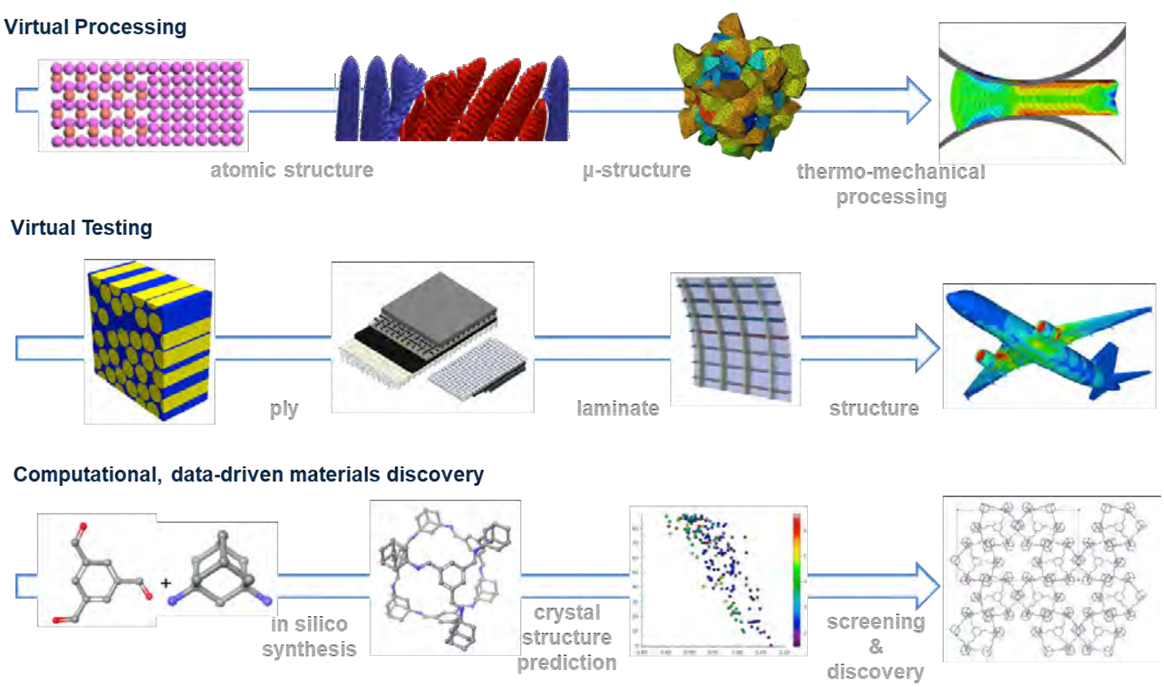
- Light (Al, Mg and Ti) metallic alloys and their composites. Ni-based superalloys. Multifunctional composite materials and structures. Materials for energy generation and storage.

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

MOAMMM / Multi-scale Optimization for Additive Manufacturing of fatigue resistant shock-absorbing MetaMaterials

Funding: European Commission/ Horizon 2020 Programme – FET Open
Partners: University of Liège (Coordinator), KU Leuven, Johannes Kepler University Linz, IMDEA Materials Institute, CIRP GmbH
Project period: 2020 - 2024
Principal Investigator: Prof. J. Segurado

The emergence of metamaterials has opened a new paradigm in designing engineering parts in which the design of full structural parts can be optimised together with the metamaterial they are locally composed of. Moreover, additional morphing at local and global scales may support their adaptation to variable loading conditions and shifted user needs. As polymeric materials can fulfil simultaneously structural mechanical and functional requirements, the combination of this design paradigm with additive manufacturing can support/generate novel applications. However, many challenges are left in order for this change of paradigm to become a reality:

- To improve metamaterial design and fabrication technique to produce damage tolerant metamaterials.
- Robust and efficient concurrent multiscale techniques should be developed as part of a multiscale optimization problem.
- Because microstructure and material properties suffer from uncertainties affecting structural responses, techniques for uncertainty quantification should be developed for this multiscale design problem.

These challenges can only be addressed by considering experimental and numerical multi-scale methods. However, current existing approaches are limited in several aspects because on the one hand of the difficulty in representing the microstructure and characterizing micro-scale constituent materials, and on the other hand in the computational cost inherent to these approaches. The overall objective of MOAMMM project is to develop a data-driven methodology relying on a structural properties-micro-structure linkage and able to design optimized shock-absorption devices based on bi-stable metamaterials and printable using additive manufacturing (see Figure 1). Targeted applications are user-optimized shock absorber devices which either potentially suffer from fatigue such as in the case of sport shoe soles or which should dissipate the maximum energy during their failure such as in the bicycle helmets.

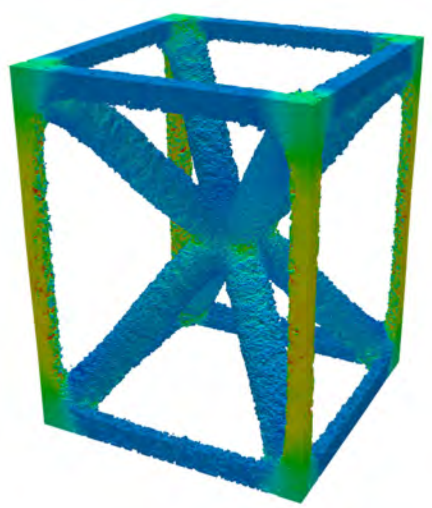


Figure 1: computational calculation performed via FFTMAD software of a tomography of lattice material made from PA12 via additive manufacturing.

Research in focus

Accelerated product development via AI-guided material design and chemical processes optimization

IMDEA Materials has know-how in developing data-driven experimentation workflows that exploit machine learning algorithms to minimize the number of experiments involved in the development of materials tuned to specific applications and/or the chemical processes governing their synthesis and scale-up. These approaches are mainly focused on the development of statistical surrogate models of experiments involved in the development of materials or processes. The high accuracy of the resulting models allows employing them in high-throughput virtual screening, often aided with efficient search algorithms, to identify optimal outcomes. The critical part of these methods are customized, problem-focused feature representations that are not only responsible to model robustness but also offer interpretability, which aids with the knowledge dissemination and the engagement with the research team responsible for the experimental verification of the optimal designs.

For more information, please contact
Dr. Maciej Haranczyk at maciej.haranczyk@imdea.org

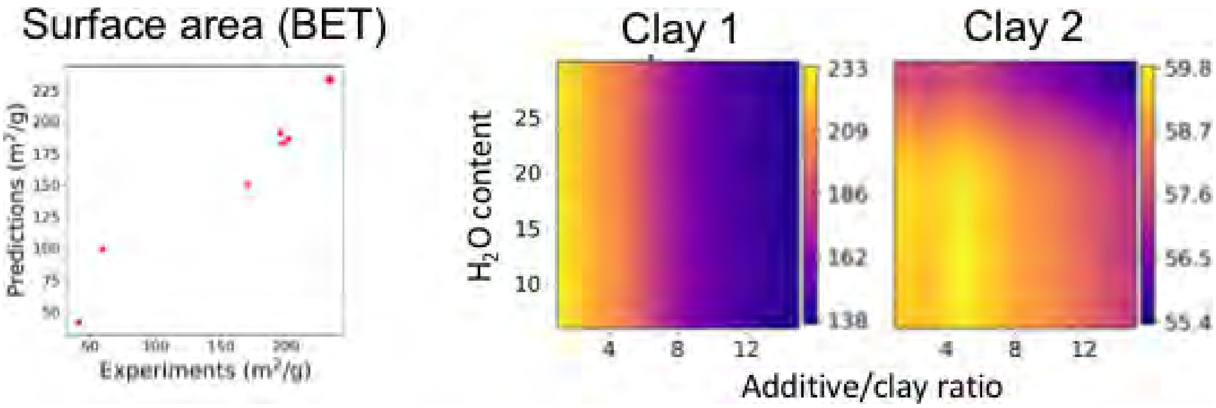


Figure 1: tuning the surface area of processed natural clays. Left –a statistical model for prediction of surface area in processed clays shows good accuracy. Right – an application of the said model in scanning the experimental parameter space to find processing conditions that maximize the surface area.

IMDEA Materials has experience in diverse cases ranging from ones such as the design of molecules and molecular fragments in ionic liquids and crystalline polymers to the tuning of processing protocols for mineral and clays-based materials (see Figure 1). This expertise can be adapted to a variety of applications regardless if the precise chemical structures of the system involved are known or not.

Predictive simulation of metal additive manufacturing. From composition and processing to mechanical properties

As part of its strategic initiative on *damage-tolerant additive manufacturing*, IMDEA Materials develops a suite of physics-based computational models and simulation tools aimed at linking processing, microstructures and properties, in order to accelerate the discovery and deployment of new alloys designed specifically for Additive Manufacturing (AM) with outstanding properties and to optimize processing conditions for AM of metals and alloys (see Figure 1).

State-of-the-art models developed and combined within this research thrust include:

- Finite Element (FE) simulation of macroscopic processing, e.g. Selective Laser Melting (SLM), in order to predict residual stresses, printed part distortion, and local thermal history used as input toward lower-scale models.
- Phase-Field (PF) modeling of microstructure formation in the melt pool in fusion-based processes, e.g. SLM, to predict grain texture and solute segregation.
- Crystal Plasticity (CP) modeling and computational homogenization to predict the mechanical response and performance (e.g. fatigue life) of complex heterogeneous microstructures.
- Computational Thermodynamics (CalPhaD) to calculate temperature-dependent thermo-physical properties, stable phases, and transformation temperatures, of complex multicomponent alloys.
- Advanced characterization methods (e.g. powder characterization, microstructure characterization, fatigue, testing, high-temperature micro/nano-mechanics, etc.) used to validate and/or calibrate models to ensure their predictive capabilities.

Ongoing activities include combining computational thermodynamics, FE process thermomechanics, PF modeling of microstructure formation, and CP for SLM of Nickel-based superalloys for high-temperature aeronautical applications; and leveraging computational thermodynamics and advanced material characterization to design compositionally/functionally graded steels and metal components via Direct Energy Deposition (DED) technology.

For more information, please contact
Prof. Javier Segurado at javier.segurado@imdea.org

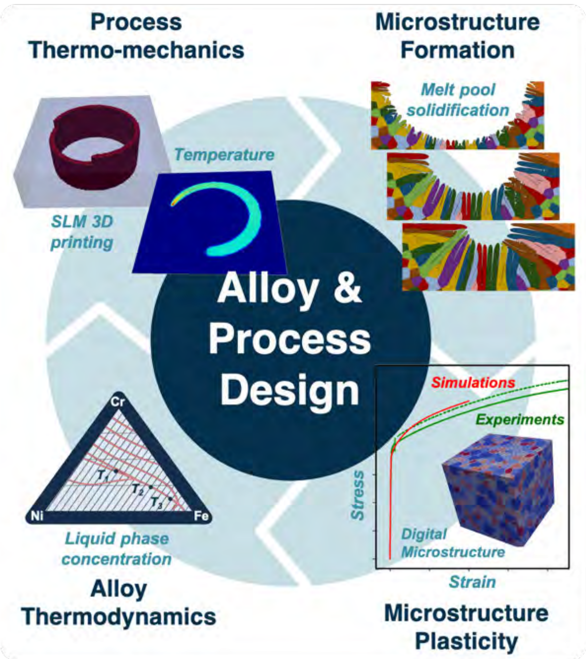
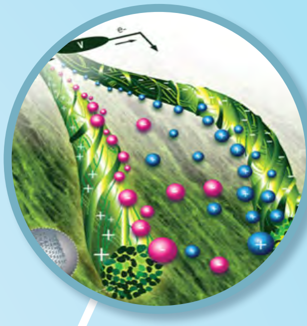


Figure1: integrated framework for the development of new alloys and processes for AM of metals.

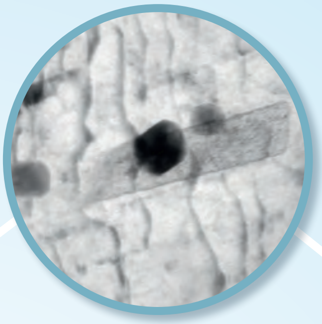
programme
Multiscale Characterisation of Materials and Processes

Goal and vision

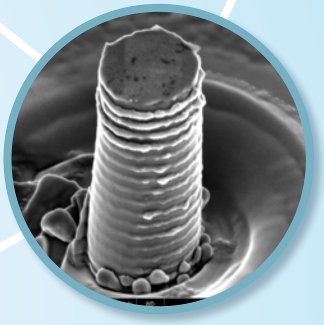
Progress in the development of new materials and processing methods can only come from a thorough understanding of microstructure evolution, either during processing or during service operation. Since the microstructural features that determine the material behaviour usually span several length scales (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.



Multifunctional Nanocomposites

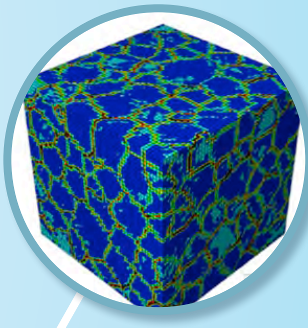


Physical Metallurgy

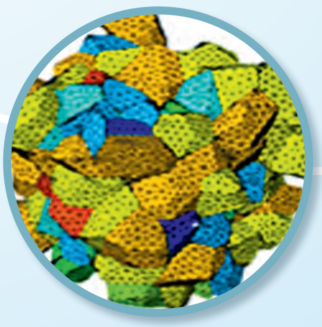


Nanomechanics

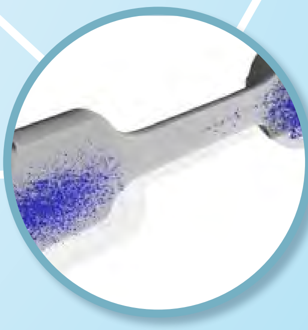
Structural Composites



Mechanics of Materials



Multiscale Materials Modelling



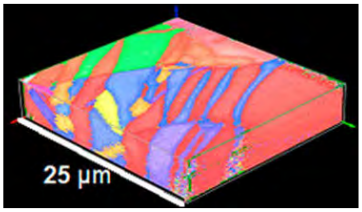
X-Ray Characterisation of Materials

Main research lines

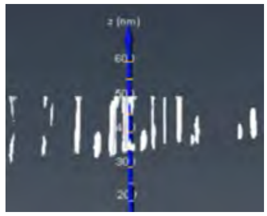
3D characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques:

- 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



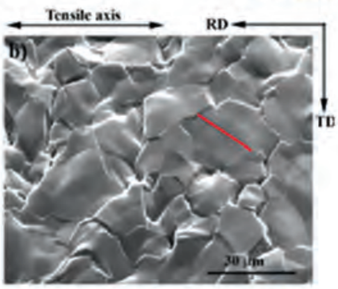
3D-TEM of Mg-Zn precipitates

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

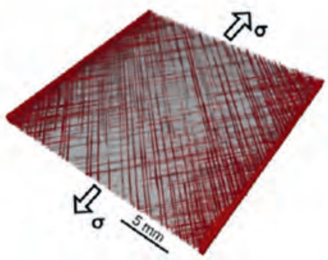
- **In-situ mechanical testing** across several length scales:
  - Tension, compression, fatigue, creep…of advanced metallic alloys and composites in the SEM and XCT.
  - Micro- and nanomechanical testing (nanoindentation, micropillar compression, microtensile testing…), including elevated temperature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

From mm....

...to nm



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

ENTENTE / European Database for Multiscale Modelling of Radiation Damage

Funding: European Commission/ EURATOM
Partners: CIEMAT (Coordinator), Bay Zoltan Nonprofit Ltd. for Applied Research (BZN), French Alternative Energies and Atomic Energy Commission (CEA), CNRS, Electricité de France (EDF), Framatome GmbH, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), IMDEA Materials Institute, Institut de Radioprotection et de Surete Nucleaire (IRSN), KTH Royal Institute of Technology in Stockholm, University of Cantabria, National Nuclear Laboratory Limited (NNL), Phimeca, SCK CEN, The University of Warwick, The University of Bristol, The Materials Performance Centre (MPC) of the University of Manchester, University of Alicante, Universitat Politècnica de Catalunya – BarcelonaTech, Technical University of Madrid, Culham Centre for Fusion Energy, UJV Rez, VTT Technical Research Centre of Finland, State Enterprise State scientific and Technical Center for nuclear and radiation safety (SSTC), Chalmers University of Technology, Central Research Institute of Electric Power Industry (CRIEPI)
Project period: 2020 - 2024
Principal Investigator: Dr. J. M. Molina-Aldareguia

ENTENTE project aims to design a new EU experimental/ modelling materials database to collect and store highly relevant data on radiation damage of Reactor Pressure Vessel (RPV) steels, according to FAIR (Findability, Accessibility, Interoperability, and Reusability) principles. The project consists of three interconnected blocks (Figure 1):

1) Database design
- Definition of new effective data formats suitable for microstructural and modelling data, and interfaces needed to ensure interoperability.
- Interface the SOTERIA platform with the ENTENTE database, so that experimental data and metadata can be retrieved and post processed in order to correctly parametrize modelling tools.

2) Advanced experiments/models
- Microstructural characterisation, linked with appropriate models, for mapping the radiation induced defects and associated strain-stress fields.
- In-depth analysis of segregation and structural, chemical nature and strength of grain boundaries to study hardening and non-hardening embrittlement.

3) Innovative data analysis and hybrid models
- Simulation tools that enable the description of radiation damage up to length and time scales that are comparable with those reached in experiments on RPV steels. Accelerated physically informed fracture laws with a reasonable predicting capability on heterogeneous microstructures.
- First application of Integrated Computational Materials Engineering (ICME) approaches to enable virtual studies of alternative neutron embrittlement scenarios.
- Machine learning and artificial neural networks approaches not only to support atomistic modelling but also to predict hardening and/or embrittlement

The exploitation of the ENTENTE database (see Figure 1), including the interface with SOTERIA platform, will allow the integrity assessment of Reactor Pressure Vessel to be improved both in a Long Term Operation (LTO) perspective and for new Gen III+ reactors.

IMDEA Materials is working on the characterization of the effect of ion irradiation induced damage on the mechanical properties of reactor pressure vessel model alloys as a function of annealing and operating temperature, using nanoindentation. Additionally, IMDEA Materials will contribute to the advanced microstructural characterization tasks, with S(TEM) characterization of deformation of ion damaged lamellae prepared by FIB.

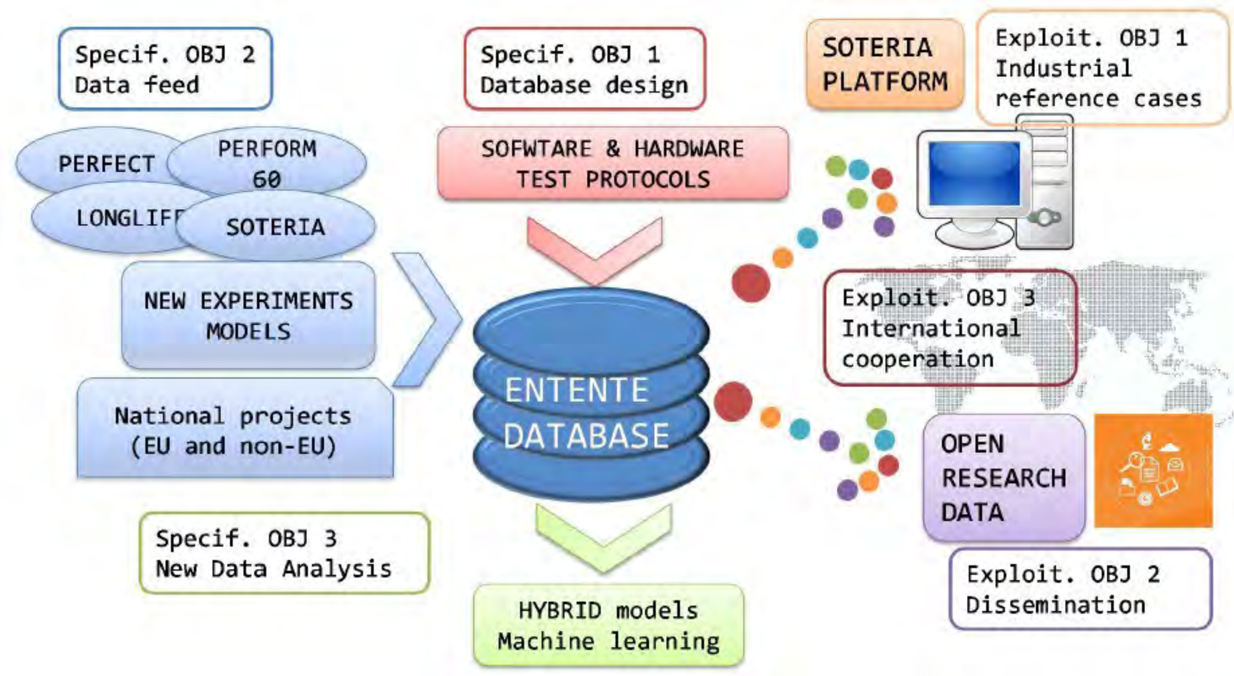
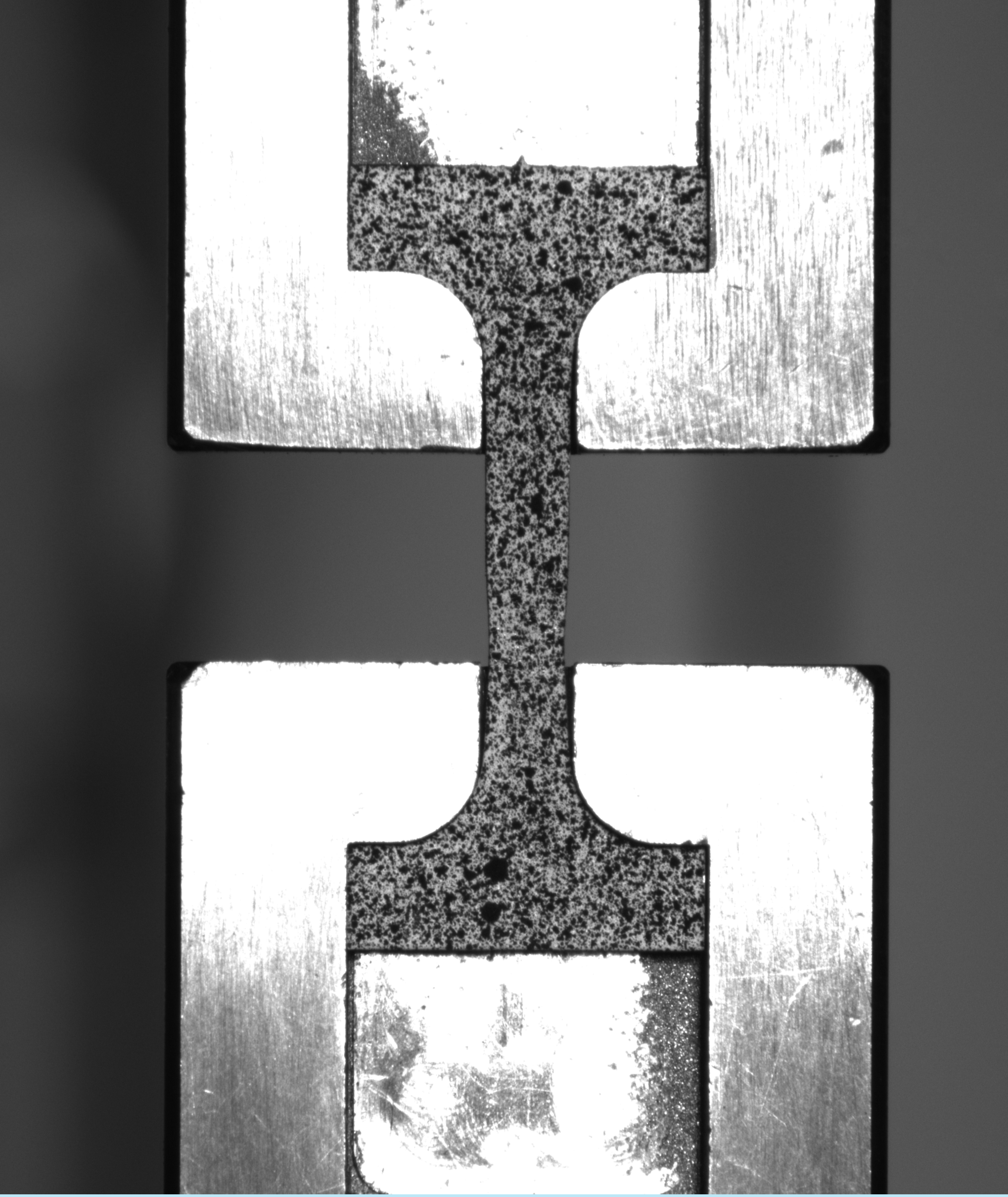


Figure 1: objectives of the ENTENTE project (Grant Agreement 900018, EURATOM)



Research in focus

Multiscale in-situ characterization of materials and processes

Current trends to reduce weight, energy consumption and improve functionality are leading to new materials with complex microstructures, whose behavior can only be understood from the synergetic contribution of processes occurring at multiple length scales (from nm to m). Examples of these materials are structural composites, duplex alloys or materials with evolving microstructures that deform by unconventional deformation mechanisms (TWIP and TRIP steels), nanoporous foams or hierarchical meta-materials produced by Additive Manufacturing. The design of new materials and their application requires a complete fundamental understanding of their behavior and *in situ* studies are crucial to achieve this.

The IMDEA Materials Institute gathers experts in advanced characterization that make use of state-of-the-art *in situ* devices (both commercial and developed in-house) to test materials under different loading configurations (tension/compression/fatigue at ambient and elevated temperature) and to physically simulate processing (e.g. solidification or resin infiltration of fiber preforms). Tests are carried out on specimens ranging in size from hundreds of nanometers to several millimeters under different characterization beams, such as Scanning Electron Microscopy (SEM), Focused Ion Beam (FIB), Transmission Electron Microscopy (TEM), as well as X-ray Computed Tomography (XCT) and X-ray diffraction (XRD), both using laboratory and synchrotron X-ray radiation. Some examples of the offered capabilities are [1, 2]:

- ***In situ* mechanical testing in the SEM and TEM at different scales (macro-micro-nano)**

In situ mechanical testing in the SEM and TEM, as shown in Figure 1, can provide information on deformation mechanisms and damage evolution in advanced metallic alloys and structural composites. This allows detecting "hot spots" in the material microstructure that can lead to damage accumulation and the final failure of engineering

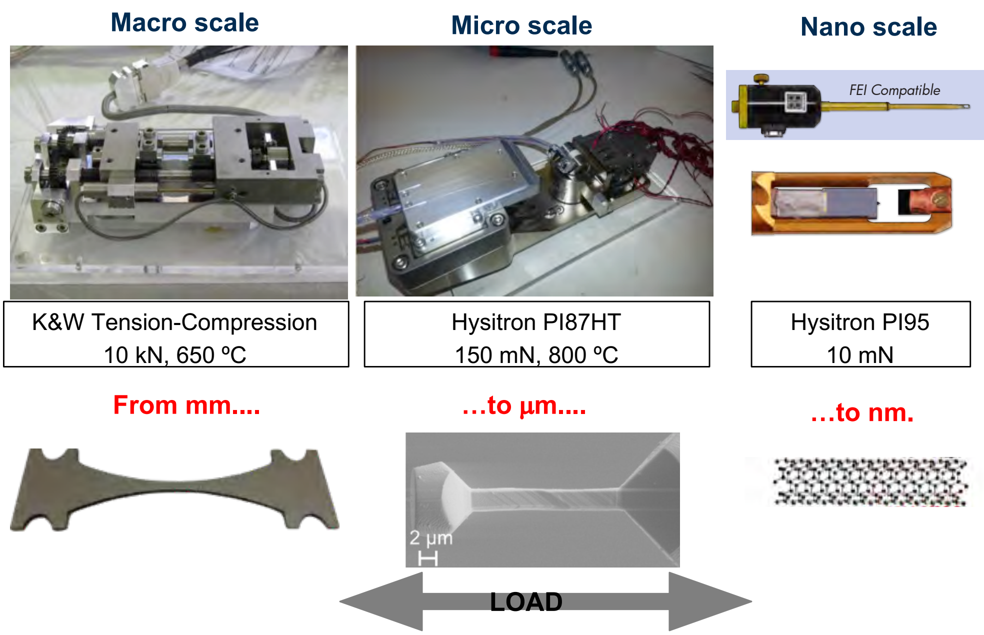


Figure 1: in situ mechanical testing at different scales in the SEM and TEM.

components. This fundamental knowledge can be used to tailor better microstructures through the control of the processing methods and to produce longer lasting products.

- ***In situ* XCT devices for processing and mechanical characterization**

Many industrial processes of engineering materials are not yet fully understood. This is also true for the mechanical behavior of many materials. One way to shed some light on the effect of the parameters affecting the processes, or the effect of the microstructure on the mechanical properties is to be able to look into the materials as the process or the mechanical deformation is occurring. This requires the use of non-destructive techniques as e.g. XCT combined with appropriate devices able to replicate the desired event. Examples of developed devices at IMDEA Materials for process replication during XCT are: a) for composite materials: devices for resin infiltration into fibers (infusion and VARTM), curing device for autoclave and out-of-autoclave processes, b) for metals and alloys: resistive furnaces for studies of directional solidification or phase formation and chemical reaction by infiltration of liquid metals into porous preform, portable induction furnaces for *in-situ* XCT and XRD heat treatments. For mechanical testing of many materials during XCT inspection, a tensile/compression/low cycle fatigue with a temperature module of up to 600ºC has been also developed at IMDEA Materials.

For more information, please contact
Dr. Jon Molina at jon.molina@imdea.org

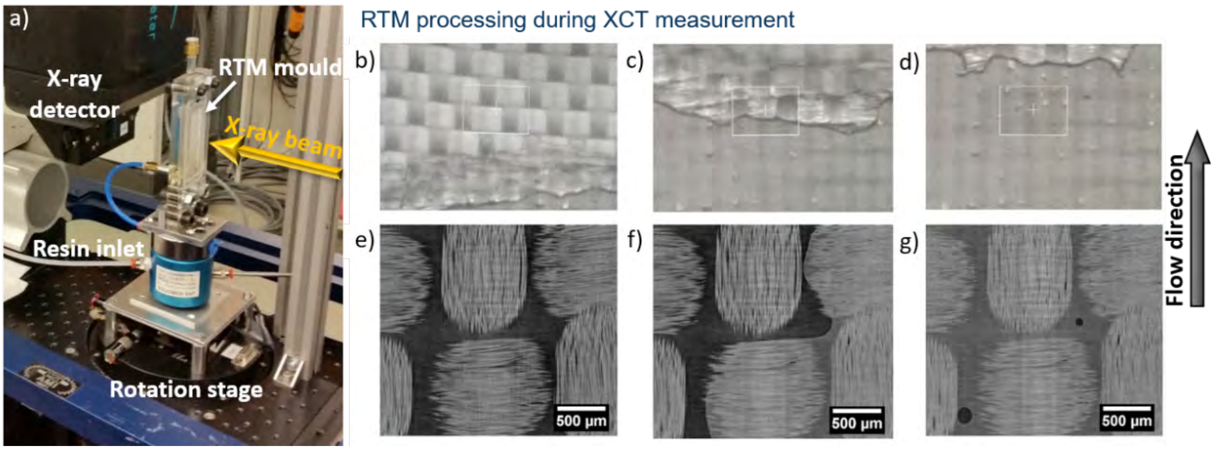


Figure 2: in situ resin transfer moulding studies by XCT. a) Experiment set-up. b) to d) video camera images of the infiltration experiment at different stages. e) to g) Tomographic cross-sections in the middle of the mould showing fiber fabrics (light-gray), resin (middle-gray) and air (dark-gray).

[1] J. Castro, F. Sket, C. González, S-XCT experimental determination of local contact angle and meniscus shape in liquid moulding of composites, **Composite Science and Technology 199**, *108362 (2020)*

[2] M. Rueda-Ruiz, M. A. Monclús, B. D. Beake, F. Gálvez, J. M. Molina Aldareguia, High strain rate compression of epoxy micropillars, **Extreme Mechanics Letters 40,** *100905 (2020*

New coatings for extreme conditions

Titanium aluminum nitrides (TiAlN) are currently the most versatile coatings in terms of performance with various applications in industry: as wear-resistant coatings for cutting tools; for increasing productivity in die casting, reducing soldering and retarding fire cracks; for plastic processing, such as injection molding and extrusion; for metal forming, like blanking, deep drawing, punching or trimming; and they are also finding applications for protecting pieces from high abrasion, like turbine blades. The industry-standard technique for the deposition of these coatings is cathodic arc deposition, although it is well known for producing porous, rough coatings with a high number of defects and particulates. Moreover, these coating typically offer a high hardness, but a limited fracture toughness, leading to relatively brittle coatings, that tend to crack along the existing defects, such as the boundaries of their columnar grains.

IMDEA Materials Institute is working in different directions to produce new coatings for extreme conditions that combine, not only a high hardness, but also a large fracture toughness. Several directions are followed for this [1, 2]:

- The exploitation of novel techniques like High-Power Impulse Magnetron Sputtering (HiPIMS), which has the potential to vastly reduce the downsides of Arc Evaporation by the application of high-energy ion bombardment over the coating surface, resulting in much denser defect-less coatings.

- The development of quaternary TiAlN coatings by the addition of other elements such as Cr, Si, Zr, B, Ni or others or the use of nanolaminated structures. In particular, a better understanding of the microstructure formation is seek with the objective of suppressing columnar growth, which is known to compromise the fracture toughness of the coatings. For instance, Figure 1 show an example on how the addition of small amounts of Ni into a TiN coating suppresses columnar growth, which has strong implications on the coating fracture resistance.

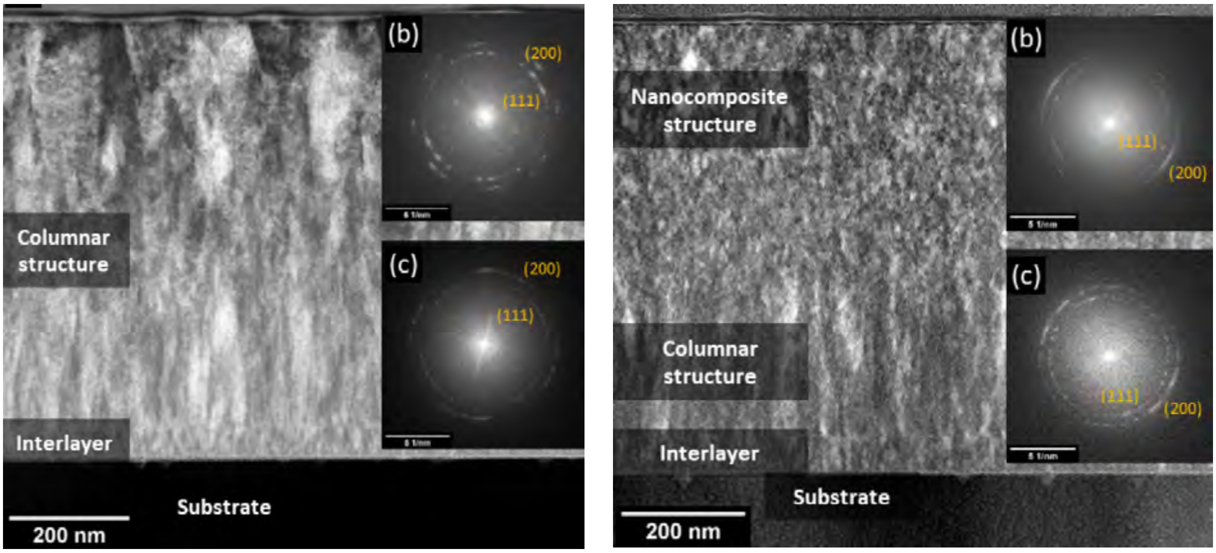


Figure 1: TEM images of the cross-sections of a (Left) a TiN coating and (Right) a TiN coating with small additions of Ni, for which the columnar growth is suppressed.

- The exploitation of novel advanced characterization techniques. Nowadays, the mechanical properties of coatings are characterized by conventional nanoindentation tests. However, IMDEA Materials is expert on the application of novel nanomechanical tests in coatings, such as high temperature nanoindentation for the determination of hardness at elevated temperature, the micropillar splitting test (Figure 2) for the determination of fracture toughness or the incremental Focused Ion Beam (FIB) milling technique for the determination of residual stresses. These techniques provide valuable fundamental information for the development of new coatings for extreme environments that cannot be obtained by conventional testing approaches.

For more information, please contact
Dr. Jon Molina at jon.molina@imdea.org

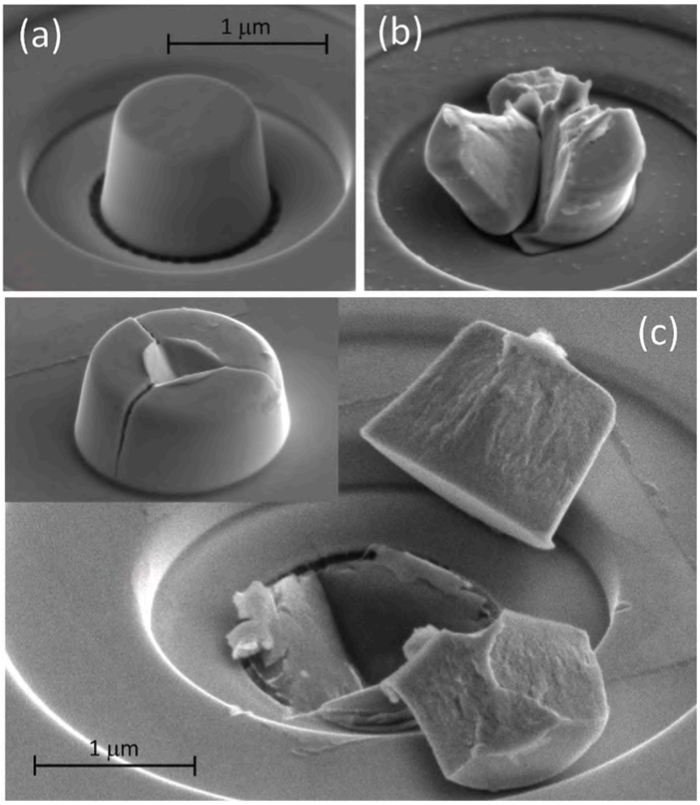


Figure 2: examples of micropillar splitting tests for the determination of the fracture toughness of coatings.

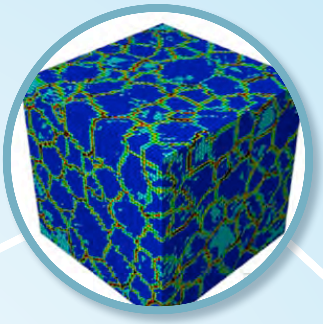
[1] *J. A. Santiago, I. Fernández-Martínez, J. C. Sánchez-López, T .C. Rojas, A. Wennber, V. Bellido-González, J. M. Molina-Aldareguia, M. A. Monclús, R. González-Arrabal, Tribomechanical properties of hard Cr-doped DLC coatings deposited by low-frequency HiPIMS.* **Surface & Coatings Technology 382,** *124899 (2020)*

[2] *I. Lopez-Cabanas, J. Llorca, R. González-Arrabal, E. I. Meletis, J. M. Molina-Aldareguia, High throughput optimization of hard and tough TiN/Ni nanocomposite coatings by reactive magnetron sputter deposition,* **Surface & Coatings Technology 418,** *127226 (2021)*

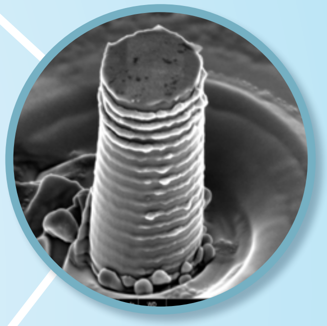
programme
Materials for Health Care

Goal and vision

Developing of novel materials-based approaches for addressing a number of challenges in medicine, ranging from treating organ/tissue damage to improving drug delivery. The programme is focused on key aspects of materials science and engineering, including chemical synthesis/modification and manufacturing of relevant materials (small molecules, polymers, biodegradable metals and composites, micro/nanoparticles, etc.), fabrication and functionalization of scaffolds (additive manufacturing, bioprinting), material characterization (microstructure, *in vitro* mechanical and chemical performance) and characterization of the biological effects and cytocompatibility of the materials using cell culture. This programme is supported by state-of-the-art new facilities for biomaterials processing and cell culture, to be fully operative in year 2021. The long-term vision is to develop collaborations with clinicians and biomedical researchers (at hospitals, research centers and industry) to enable translational research.



Mechanics
of Materials



Nanomechanics

Structural
Composites

Main research lines

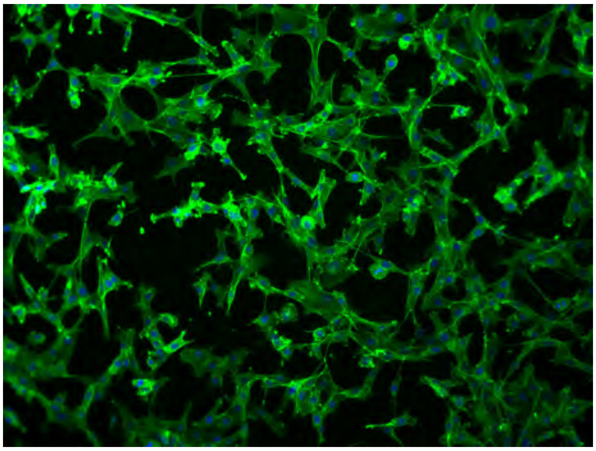
Additive manufacturing of biodegradable scaffolds (metallic, polymeric and composites) for tissue engineering (bone, cartilage, skin).

Biofunctionalization and surface modification on materials with molecules (proteins, peptides, grow factors, drugs) to improve the performance of materials for biological applications and medical devices.

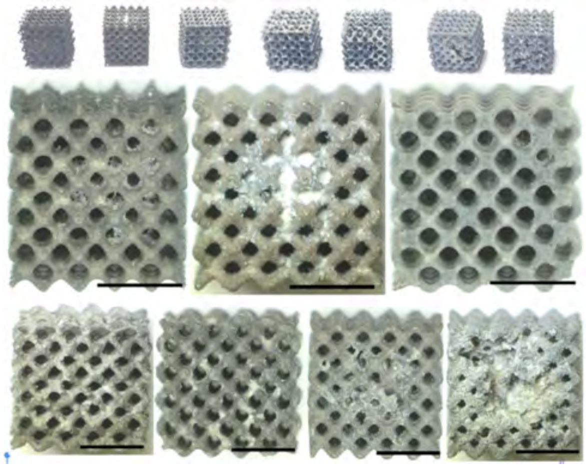
Mechanotransduction: effect of mechanical and electrical stimuli on biological actions

Manufacturing and application of **nanoparticles for drug delivery, disease treatment and antimicrobial activity**.

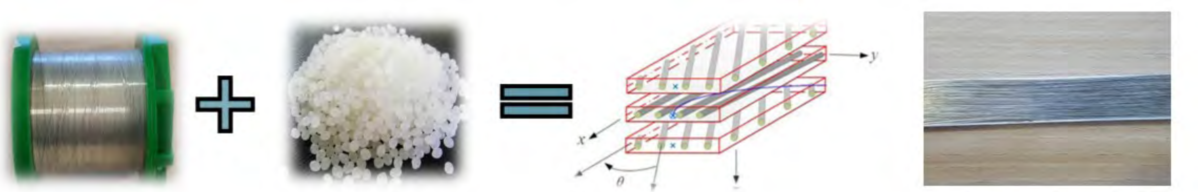
Characterization of cytocompatibility and biological functionality *in vitro*.



Pre-osteoblast MC3T3-E1 attached on Poly(DL-lactide) medical grade polymer used in the manufacturing of 3D scaffolds for bone regeneration. In blue the nucleus and in green the cytoskeleton. Winner imaging contest 2021. Characterization



3D printed Mg scaffolds for bioresorbable bone implants



PLA-Mg fiber", con pie de figura "Bioresorbable PLA/Mg fiber composite plate for biomedical applications

Projects in focus

BioImplant ITN / European Training Network to develop Improved Bioresorbable Materials for Orthopaedic and Vascular Implant Applications

Funding: European Commission, Horizon 2020 Programme, Marie Skłodowska-Curie Actions – Innovative Training Networks (Grant Agreement 813869)
Partners: National University of Ireland Galway (coordinator), IMDEA Materials Institute, The Queens University of Belfast, RWTH Aachen, Boston Scientific Ltd., 3D Technology, Vascular Flow Technologies, Meotec and ITA Textil Technologie Transfer
Project period: 2018 – 2022
Principal Investigator: Prof. J. Llorca

BioImplant ITN is a multidisciplinary training network for 12 predoctoral researchers in the area of bioabsorbable medical implant development. The network is formed by 4 academic institutions and 5 companies. The research vision of the project (Figure 1) is to use an integrative approach that combines polymer-, metal- and ceramic-based bioabsorbable materials, to deliver functionally superior bioabsorbable materials with enhanced mechanical behaviour and controllable degradation profiles. The successful development of these materials has the potential to form the basis for the next-generation of medical implants.

IMDEA Materials is the host of three researchers working on the development of bioabsorbable scaffolds for bone regeneration and growth from textile composites of poly-lactic acid and poly-lactic acid reinforced with Mg fibers and/or Mg particles. The scaffolds are manufactured using different techniques (additive manufacturing by fused filament deposition, hot pressing) depending on the application, the material, and their mechanical properties. Degradation rates (Figure 2) in simulated body fluids and cytocompatibility are determined to assess the viability for in vivo studies in animal models.

Figure 1: research vision of the BioImplant ITN project: integrative approach that combines polymer-, metal- and ceramic-based bioabsorbable materials.

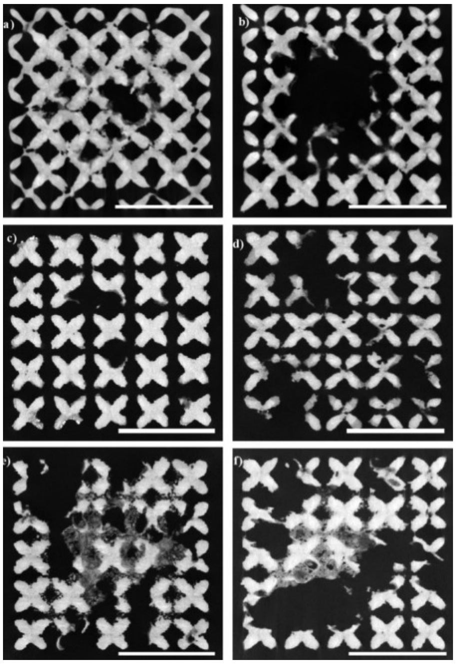


Figure 2: corrosion behaviour of WE43 Mg alloy scaffolds fabricated by laser powder bed fusion.

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, Physical Metallurgy

Ph.D. in Materials Science from Complutense University of Madrid. Spain

Research Interests

Applied and fundamental work on the processing, characterisation and mechanical behaviour of advanced metallic materials for automotive, energy and biomedical applications; design of novel alloys for additive manufacturing; in situ investigation of the deformation and recrystallization mechanisms of light and high temperature metals; fabrication of novel metallic phases with improved mechanical and functional properties by non-equilibrium processing.

Prof. Javier LLorca

Scientific Director, Mechanics of Materials

Ph.D. in Materials Science from Technical University of Madrid. Spain

Professor of Materials Science, Technical University of Madrid

Research Interests

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

Prof. Carlos González

Senior Researcher, Structural Composites

Ph.D. in Materials Science from Technical University of Madrid. Spain

Professor of Materials Science, Technical University of Madrid

Research Interests

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

Dr. Jon M. Molina-Aldareguía

Senior Researcher, Micromechanics and Nanomechanics

Ph.D. in Materials Engineering from Cambridge University. United Kingdom

Research Interests

Micro- and nano-mechanical testing and advanced focused-ion beam and electron microscopy analysis of advanced structural materials; microstructural and mechanical characterisation of thin-films; mechanical testing inside the scanning and transmission electron microscopes.

Dr. Javier Segurado

Senior Researcher, Multiscale Materials Modelling

Ph.D. in Materials Engineering from Technical University of Madrid. Spain

Associate Professor of Materials Science, Technical University of Madrid

Research Interests

Multiscale modelling of structural materials; physically-based models to simulate the mechanical behaviour of metals at different length scales: molecular dynamics, discrete dislocation dynamics and single-crystal plasticity models; computational homogenization models and concurrent multiscale techniques for polycrystalline materials; and development of computational micromechanics strategies to simulate the mechanical behaviour until failure of both particle- and fibre-reinforced composites.

Dr. Juan José Vilatela

Senior Researcher, Multifunctional Nanocomposites

Ph.D. in Materials Science from University of Cambridge. United Kingdom

Research Interests

Development of macroscopic materials made up of nanobuilding blocks in a way that the unique properties at the nanoscale are preserved through the assembly process and a new generation of high-performance engineering materials is produced. Central to this work is a process to make continuous macroscopic fibres made up of CNTs. Study of their hierarchical structures by advanced X-ray techniques, reinforcement at multiple length-scales and the electrochemical interactions of CNT fibres with liquids and polymers. This research has helped establish the unique combination of properties of CNT fibres, and is enabling the fabrication of multifunctional composites that can store and harvest energy or have sensing functions.

Prof. José Manuel Torralba

Senior Researcher, Powder Metallurgy

Ph.D. in Metallurgy from Technical University of Madrid. Spain. PhD in Armament Engineer from the Polytechnic School of Elche. Spain

Research Interests

Powder metallurgy, powder development, characterization and advanced consolidation methods (field assisted sintering, metal injection moulding, additive manufacturing…) in particular. He has worked with most families of materials in powder metallurgy, such as low-alloyed steels, special steels, hardmetals, superalloys, light alloys and metal matrix composites, high entropy alloys, etc…

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.

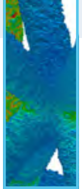
Dr. Ruben D. Costa

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); non-equilibirum 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

Dr. Álvaro Ridruejo
Visiting Scientist

Ph.D. in Material Science from the Technical University of Madrid. Spain

Associate Professor of Material Science at the Technical University of Madrid. Spain

Dr. Mutasem Shehadeh
Visiting Researcher

Ph.D. in Mechanical Engineering from Washington State University. USA

Associate Professor of Mechanical Engineering at the American University of Beirut. Lebanon

Lights in the dark in the data center.
Winner imaging contest 2021. Open subjet

annex

1. R&D projects and contracts

1.1. European R&D Projects (European Commission)

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. J. J. Vilatela

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. S. Milenkovic and Dr. C. Cepeda

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. I. Sabirov

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. J. Llorca

Title/Acronym: Structural energy harvesting composite materials/STEM
Partners: IMDEA Materials Institute
Period: 2016 – 2021
Funding Institution/Programme: European Commission/Horizon 2020 Programme – ERC Starting Grant
Principal Investigator: Dr. J. J. Vilatela

Title/Acronym: European Database for Multiscale Modelling of Radiation Damage/ ENTENTE
Partners: CIEMAT (Coordinator), Bay Zoltan Nonprofit Ltd. for Applied Research (BZN), French Alternative Energies and Atomic Energy Commission (CEA), CNRS, Electricité de France (EDF), Framatome GmbH, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), IMDEA Materials Institute, Institut de Radioprotection et de Surete Nucleaire (IRSN), KTH Royal Institute of Technology in Stockholm, University of Cantabria, National Nuclear Laboratory Limited (NNL), Phimeca, SCK CEN, The University of Warwick, The University of Bristol, The Materials Performance Centre (MPC) of the University of Manchester, University of Alicante, Universitat Politècnica de Catalunya – BarcelonaTech, Technical University of Madrid, Culham Centre for Fusion Energy, UJV Rez, VTT Technical Research Centre of Finland, State Enterprise State scientific and Technical Center for nuclear and radiation safety (SSTC), Chalmers University of Technology, Central Research Institute of Electric Power Industry (CRIEPI),
Period: 2020 - 2024
Funding Institution/Programme: European Commission/EURATOM
Principal Investigators: Dr. J. M. Molina Aldareguia

Title/Acronym: Engineered Artificial Proteins for Biological Light-Emitting Diodes/ ARTIBLED
Partners: IMDEA Materials Institute (Coordinator), CSIC, Universita Degli Studi di Torino, ABIEL, CIC-biomaGUNE, TU Graz, Technical University of Munich
Period: 2020 - 2023
Funding Institution/Programme: European Commission/Horizon 2020 Programme – FET Open
Principal Investigator: Dr. R. Costa

Title/Acronym: Multi-scale Optimization for Additive Manufacturing of fatigue resistant shock-absorbing MetaMaterials/MOAMMM
Partners: University of Liège (Coordinator), KU Leuven, Johannes Kepler University Linz, IMDEA Materials Institute, CIRP GmbH
Period: 2020 - 2024
Funding Institution/Programme: European Commission/Horizon 2020 Programme – FET Open
Principal Investigator: Prof. J. Segurado

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. A. Mikhalchan; Supervisor: Dr. J. J. Vilatela

Title/Acronym: new circular polarized light-emitting electromechanical cells/ NEWCPLECS
Partners: IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - IF
Principal Investigator: Dr. J. J. Fernández-Cestau; Supervisor: Dr. R. Costa

Title/Acronym: Creating an infrastructure for the numerical exploration of metallurgical alloys/CINEMA
Partners: IMDEA Materials Institute
Period: 2019 – 2021
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions – IF
Principal Investigator: Dr. D. Tourret; Supervisor: Prof. J. Segurado

Title/Acronym: Chiral flame retardant materials: Design, Synthesis and study of chirality-flame retardancy relationship/REMES
Partners: IMDEA Materials Institute
Period: 2019 – 2021
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions – IF
Principal Investigator: Dr. J. Cui; Supervisor: Dr. D-Y Wang

Title/Acronym: Multiscale Analysis of Fatigue in Mg Alloys/MAFMA
Partners: IMDEA Materials Institute
Period: 2019 – 2021
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions – IF
Principal Investigator: Dr. A. Ma; Supervisor: Prof. J. Llorca

Title/Acronym: Multiscale analysis of precipitate in al-cu alloys/MAPAA
Partners: IMDEA Materials Institute
Period: 2020 – 2022
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions – IF
Principal Investigator: Dr. S. Liu; Supervisor: Prof. J. Llorca

Title/Acronym: Tailored Lightweight Sandwich Composites with Multifunctional Properties and Good Designability/TESCOM
Partners: IMDEA Materials Institute
Period: 2020 – 2022
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions – IF
Principal Investigator: Dr. X. Lin; Supervisor: Dr. D-Y Wang

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. J. M. Molina-Aldareguia, Prof. C. González and Dr. F. Sket

Title/Acronym: European Training Network to develop Improved Bioresorbable Materials for Orthopaedic and Vascular Implant Applications/BioImplant ITN
Partners: National University of Ireland Galway (Coordinator), IMDEA Materials Institute, The Queens University of Belfast, RWTH Aachen, Boston Scientific Ltd., 3D Technology, Vascular Flow Technologies, Meotec and ITA Textil Technologie Transfer
Period: 2018 - 2022
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - ITN - EID
Principal Investigator: Prof. J. Llorca

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. J. P. Fernández

Title/Acronym: Silicon nanowire fabrics for high energy density batteries/SiNERGY
Partners: IMDEA Materials Institute
Period: 2020 - 2022
Funding Institution/Programme: European Commission/Horizon 2020 Programme – ERC Proof of Concept
Principal Investigator: Dr. J. J. Vilatela

Title/Acronym: Development of new martensitic stainless steels for automotive lightweight structural applications/QPINOX
Partners: Centro Sviluppo Materiali (Coordinator), Technical University of Delft, IMDEA Materials Institute, ACERINOX Europe
Period: 2019 – 2022
Funding Institution/Programme: European Commission/Research Fund for Coal and Steel (RFCS)
Principal Investigators: Dr. I. Sabirov and Dr. J. M. Molina-Aldareguia

Title/Acronym: Design of Lightweight Steels for Industrial Applications/DELIGHTED
Partners: IMDEA Materials Institute (Coordinator), Ghent University, Ocas NV, Politecnico di Milano, Max Planck Institute for Iron Research
Period: 2020 - 2023
Funding Institution/Programme: European Commission/Research Fund for Coal and Steel (RFCS)
Principal Investigator: Dr. I. Sabirov

1.2. Other International R&D Projects

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)/Industrial Fellowships
Principal Investigator: Pof. J. Segurado

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. J. J. Vilatela

Title/Acronym: Multiscale virtual testing capability for composites/MUVITCAPCOM
Partners: IMDEA Materials Institute
Period: 2019 – 2022
Funding Institution/Programme: Air Force Office of Scientific Research (AFOSR)
Principal Investigator: Prof. C. González

1.3. National R&D Projects

Title/Acronym: Excellence Unit María de Maeztu/MdM 2018
Partners: IMDEA Materials Institute
Period: 2019 – 2023
Funding Institution/Programme: Spanish Ministry of Science, Innovation and Universities (MCIU)/Severo Ochoa - María de Maeztu
Principal Investigator: Prof. J. Llorca

Title/Acronym: Ultrafine eutectics by laser additive manufacturing/ELAM
Partners: German Aerospace Research Center (DLR, 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
Principal Investigator: Dr. F. Sket and Dr. S. Milenkovic

UNIT OF EXCELLENCE MARÍA DE MAEZTU

GOBIERNO DE ESPAÑA | MINISTERIO DE CIENCIA E INNOVACIÓN | AGENCIA ESTATAL DE INVESTIGACIÓN

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
Principal Investigator: Prof. I. Romero

Title/Acronym: Advanced materials and nanomaterials Spanish technological platform/ MATERPLAT Partners: IMDEA Materials Institute (Technical Secretariat)
Period: 2019 – 2020
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
Coordinator: Miguel Ángel Rodiel

Title/Acronym: Red españOla SimulAción muLtiescala dE materialeS/ROSALES
Partners: Multiple partners coordinated by CIEMAT (Coordinator)
Period: 2020 - 2021
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. Networks of Excellence
Principal Investigator: Prof. J. Llorca

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
Principal Investigators: Prof. I. Romero, Prof. J. Segurado and Dr. D. Tourret

Title/Acronym: Development of multi-material and multifunctional 3D parts through additive manufacturing assisted by intelligent material and process design/MULTI-FAM
Partners: Arcelor Mittal (Coordinator), AIMEN, IMDEA Materials Institute
Period: 2020 - 2022

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
Principal Investigators: Dr. I. Sabirov and Dr. D. Tourret

Title/Acronym: Quest for safe and sustainable batteries using Na-ion, Mg and hybrid concepts/NAMBAT
Partners: University of Córdoba (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
Principal Investigators: Dr. V. Etacheri and Dr. M. Haranczyk

Title/Acronym: Design of electron transfer in semiconductor-dye hybrid nanoparticles for low-temperature solar cells/HYNANOSC
Partners: Universidad de Alicante (Coordinator), IMDEA Materials Institute
Period: 2019 - 2021
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness (MINECO)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigators: Dr. R. Costa and Dr. J. Vilatela

Title/Acronym: Additive manufacturing of fibre reinforced thermoplastic composites for transports, healthcare and sports/ADDICOMP
Partners: University of Mondragon (Coordinator), IMDEA Materials Institute, University of Girona
Period: 2019 – 2021
Funding Institution/Programme: Spanish Ministry of Science, Innovation and Universities (MCIU)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigator: Dr. J. P. Fernández

Title/Acronym: Grain Boundaries in Hexagonal microstructures: Linking processing and properties in lightweight structural alloys - HexaGB
Partners: IMDEA Materials Institute (Coordinator), Technical University of Madrid
Period: 2019 – 2021
Funding Institution/Programme: Spanish Ministry of Science, Innovation and Universities (MCIU)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigator: Dr. D. Tourret

Title/Acronym: Microstructure-topology-mechanical properties relationship of Mg-based scaffolds fabricated by 3D printing for biomedical applications/TOPOMAG-3D
Partners: IMDEA Materials Institute
Period: 2020 - 2023
Funding Institution/Programme: Spanish Ministry of Science, Innovation and Universities (MCIU)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigators: Dr. J. M. Molina-Aldareguia, Dr. F. Sket

Title/Acronym: Multiscale design of Mg alloys with high strength and ductility for sustainable transport/ENLIGHTED
Partners: IMDEA Materials Institute
Period: 2020 - 2023
Funding Institution/Programme: Spanish Ministry of Science, Innovation and Universities (MCIU)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigators: Dr. M. T. Pérez-Prado and Dr. S. Milenkovic

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. R. Costa

1.4. Regional R&D Projects

Title/Acronym: Experimental characterization and numerical analysis of composite materials under thermal and environmental aging
Partners: HEXCEL Composites and IMDEA Materials Institute
Period: 2018 – 2021
Funding Institution/Programme: Regional Government of Madrid/Industrial Doctorate
Doctoral Researcher: Iker Lizarralde
Principal Investigator and Supervisor: Prof. C. González

Title/Acronym: New generation of hard, tough and high temperature resistant multilayer coatings deposited by PVD/HiPIMS/MULTIDUR
Partners: Nano4Energy and IMDEA Materials Institute
Period: 2019 – 2022
Funding Institution/Programme: Regional Government of Madrid/Industrial Doctorate
Doctoral Researcher: Álvaro Méndez
Principal Investigators and Supervisors: Dr. J. M. Molina-Aldareguia and Dr. M. Monclús

Title/Acronym: Accelerated development of special clays for adsorption of organic compounds by incorporation of 'Big Data' and material modelling techniques
Partners: TOLSA and IMDEA Materials Institute
Period: 2019 – 2022
Funding Institution/Programme: Regional Government of Madrid/Industrial Doctorate
Doctoral Researcher: Giulia Lo Dico
Principal Investigator and Supervisor: Dr. M. Haranczyk

Title/Acronym: Improvement of the 3D Metal Jet Part Quality through print mode development supported by HRXCT characterization of the printed parts
Partners: HP Printing and Computing Solutions and IMDEA Materials Institute
Period: 2020 - 2023
Funding Institution/Programme: Regional Government of Madrid/Industrial Doctorate
Doctoral Researcher: Sergi Bafaluy Ojea
Principal Investigator and Supervisor: Dr. M. T. Pérez-Prado

Title/Acronym: Smart manufacturing of advanced materials for transport, energy and health applications/MAT4.0-CM
Partners: IMDEA Materials Institute (Coordinator), National Centre of Metallurgical Research (CENIM-CSIC), Carlos III University of Madrid, Technical University of Madrid, FIDAMC, Hospital La Paz Institute for Health Research (IdiPAZ)
Period: 2019 – 2023
Funding Institution/Programme: Regional Government of Madrid/Technologies
Principal Investigator: Dr. J. M. Molina-Aldareguia

Title/Acronym: New generation of multifunctional materials for artificial photosynthesis/FotoArt-CM
Partners: IMDEA Energy Institute (Coordinator), IMDEA Materials Institute, Centre of Astrobiology (CSIC-INTA), IMDEA Nanoscience Institute, Autonomous University of Madrid, National Centre of Metallurgical Research (CENIM-CSIC)
Period: 2019 – 2023
Funding Institution/Programme: Regional Government of Madrid/Technologies
Principal Investigator: Dr. J. J. Vilatela

Title/Acronym: Advanced manufacturing technologies for the new generation of composite materials/TEMACON
Partners: Airbus Operations (Coordinator), Zinkcloud, Obuu Tech, FIDAMC, IMDEA Materials Institute
Period: 2019 – 2022
Funding Institution/Programme: Regional Government of Madrid/Open Innovation Hubs
Principal Investigator: Prof. C. González

1.5. Privately-funded R&D Projects

Title/Acronym: Development of an unmanned aerial vehicle with maritime capabilities/AUS
Company: ALPHA UNMANNED SYSTEMS and IMDEA Materials Institute
Period: 2020
Principal Investigator: Dr. M. T. Pérez-Prado

Title/Acronym: Mechanical strength of expanded junctions/UNIEXTEST
Company: ENUSA
Period: 2018-2020
Principal Investigators: Dr. C. Cepeda and Dr. M. T. Pérez Prado

Title/Acronym: High temperature miniature mechanical testing rig for synchrotron tomography/MACHSYNCH
Company: German Aerospace Research Center DLR
Period: 2018-2020
Principal Investigator: Dr. F. Sket

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

Title/Acronym: Advanced characterization of high temperature metallic parts fabricated by additive manufacturing/JANO
Company: ITP Aero
Period: 2019-2020
Principal Investigators: Dr. M. T. Pérez-Prado and Dr. F. Sket

Title/Acronym: Development of high performance hydromagnesite-based fillers to polymers/HIGHFILL
Company: Liaoning Jinghua New Materials
Period: 2019-2020
Principal Investigator: Dr. D-Y Wang

Title/Acronym: CAPSUL Integration in DIGIMAT
Company: MSC Software Belgium SA - e-Xstream
Period: 2019-2020
Principal Investigator: Prof. J. Segurado

Title/Acronym: Evaluation of damage made by ballast impact in composite materials/BINOMIAL
Company: Patentes TALGO
Period: 2019-2020
Principal Investigator: Prof. C. González

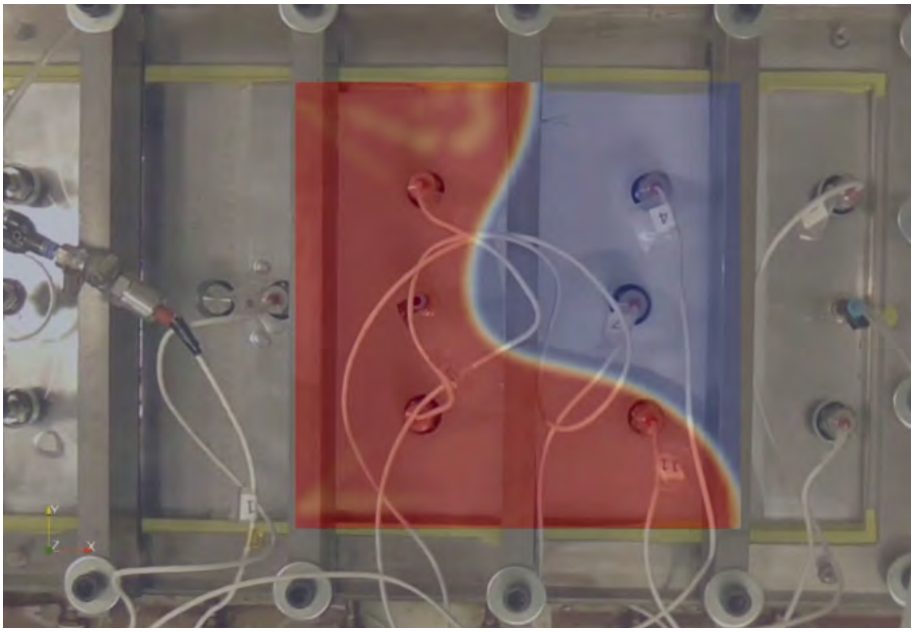
Title/Acronym: Superalloys for additive manufacturing/SAM
Company: RENISHAW Ibérica
Period: 2018-2020
Principal Investigators: Dr. M. T. Pérez-Prado and Prof. J. Llorca

Title/Acronym: Development of a novel non-halogenated, REACh compliant FR system for pressure sensitive adhesives/FRANK
Company: TESA SE
Period: 2018-2021
Principal Investigator: Dr. D-Y Wang

Title/Acronym: Development of eco-friendly high performance sepiolite based polymer composites/SEPICOM
Company: TOLSA
Period: 2020 - 2021
Principal Investigator: Dr. D-Y Wang

Title/Acronym: High-performance CNT fibre development through mechanical study of CNT bundles/NANOBUNDLE
Company: TOYOTA MOTOR EUROPE
Period: 2020
Principal Investigator: Dr. J. J. Vilatela

Title/Acronym: Study on biobased wood fibre reinforced polymer composites/ BIOCOMPOSITE
Company: University of Strathclyde Glasgow
Period: 2020
Principal Investigator Dr. D-Y Wang



Title/Acronym: Eco-friendly Fire Retardant Materials as Fireproof Coating/FIRECOAT
Company: Zhejiang RUICO New Material
Period: 2019-2020
Principal Investigator: Dr. D-Y Wang

1.6. Licenses

VIPER - Virtual Ply Property Predictor
Licensors: IMDEA Materiales Institute
Licensee: University of North Texas (UNT)
Period: 2020 – 2023
Principal Investigator: Prof. Carlos Daniel González

2. Fellowships

2.1. International

Programme: China Scholarship Council fellowships
Project: Atomistic modelling of solid-liquid interfaces in metallic alloys
Period: 2019-2021
Funding Institution: China Scholarship Council
W. Qian

Programme: China Scholarship Council fellowships
Project: Kinetics of magnesium alloys
Period: 2015-2020
Funding Institution: China Scholarship Council
N. Li

Programme: China Scholarship Council fellowships
Project: Polymer composites and nanocomposites
Period: 2015-2020
Funding Institution: China Scholarship Council
L. Zhang

Programme: China Scholarship Council fellowships
Project: High strain rate mechanical behaviour of advanced high strength steels
Period: 2016-2020
Funding Institution: China Scholarship Council
P. Xia

Programme: China Scholarship Council fellowships
Project: Multifunctional graphene thermoplastic composite materials
Period: 2016-2020
Funding Institution: China Scholarship Council
Y. Ou

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: Eco-friendly fire retardant coating
Period: 2016-2021
Funding Institution: China Scholarship Council
C. Fu

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

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

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

Programme: China Scholarship Council fellowships
Project: High performance polymer nanocomposites
Period: 2019-2023
Funding Institution: China Scholarship Council
X. Li

Programme: China Scholarship Council fellowships
Project: Development of high strength, high ductility magnesium alloys
Period: 2019-2022
Funding Institution: China Scholarship Council
X. Jin

Programme: China Scholarship Council fellowships
Project: New ideas on the investigation of mechanical properties of flame retardant composites under fire conditions
Period: 2020-2024
Funding Institution: China Scholarship Council
X. Ao

2.2. National

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

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

Programme: Ramón y Cajal
Period: 2018-2020
Funding Institution: Spanish Ministry of Economy, Industry and Competitiveness
Dr. R. Costa

Programme: Ramón y Cajal
Period: 2020-2025
Funding Institution: Spanish Ministry of Science and Innovation
Dr. F. Sket

Programme: Ramón y Cajal
Period: 2020-2025
Funding Institution: Spanish Ministry of Science and Innovation
Dr. V. Etacheri

Programme: Training University Lecturers (FPU)
Period: 2019-2022
Funding Institution: Spanish Ministry of Science, Innovation and Universities
C. Galera

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

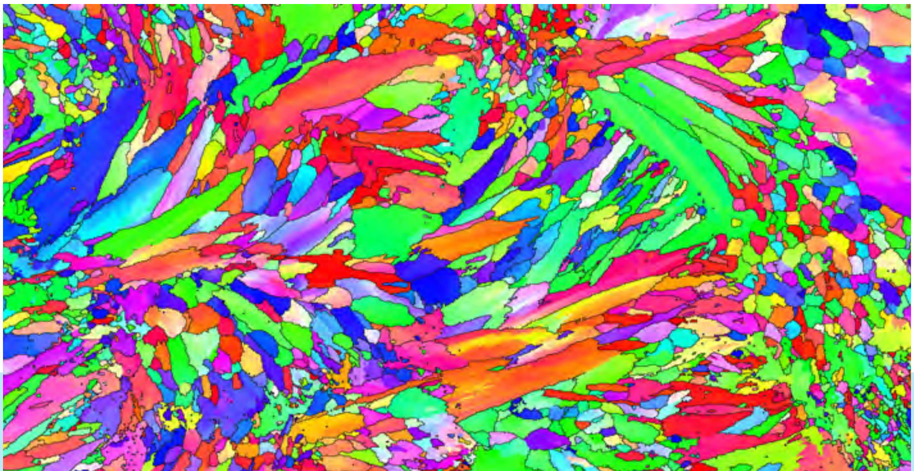
Programme: Training University Lecturers (FPU)
Period: 2016-2020
Funding Institution: Spanish Ministry of Education, Culture and Sport
B. Bellón

Programme: Training University Lecturers (FPU)
Period: 2020-2024
Funding Institution: Spanish Ministry of Universities
C. Martínez

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

Programme: Predoctoral Fellowships
Period: 2018-2022
Funding Institution: Spanish Ministry of Science, Innovations and Universities
C. Gutierrez

Programme: Predoctoral Fellowships
Period: 2020-2024
Funding Institution: Spanish Ministry of Science and Innovation
E.Kazemi



Programme: Predoctoral Fellowships
Period: 2020-2024
Funding Institution: Spanish Ministry of Science and Innovation
O. Contreras

Programme: Youth Employment Programme
Period: 2019-2021
Funding Institution: Spanish Ministry of Science, Innovations and Universities
J. de la Vega

Programme: Youth Employment Programme
Period: 2019-2021
Funding Institution: Spanish Ministry of Science, Innovations and Universities
D. González

Programme: Youth Employment Programme
Period: 2019-2021
Funding Institution: Spanish Ministry of Science, Innovations and Universities
A. Yusuf

Programme: Youth Employment Programme
Period: 2019-2021
Funding Institution: Spanish Ministry of Science, Innovations and Universities
S. Rodríguez

2.3. Regional

Programme: Talent Attraction Programme – Modality 1
Period: 2017-2020
Funding Institution: Madrid Regional Government
Dr. R. Costa

Programme: Talent Attraction Programme – Modality 1
Period: 2017-2020
Funding Institution: Madrid Regional Government
Dr. V. Etacheri

Programme: Talent Attraction Programme – Modality 1
Period: 2018-2022
Funding Institution: Madrid Regional Government
Dr. A. Ma

Programme: Talent Attraction Programme – Modality 2
Period: 2019-2020
Funding Institution: Madrid Regional Government
Dr. S. Liu

Programme: Talent Attraction Programme – Modality 2
Period: 2018-2020
Funding Institution: Madrid Regional Government
Dr. M. Vila

Programme: Youth Employment Programme/Predoctoral Fellowships
Period: 2019-2020
Funding Institution: Madrid Regional Government
A. Doñoro

Programme: Youth Employment Programme/Research assistants and laboratory technicians
Period: 2020-2022
Funding Institution: Madrid Regional Government
J. García

Programme: Youth Employment Programme/Research assistants and laboratory technicians
Period: 2020-2022
Funding Institution: Madrid Regional Government
A. León

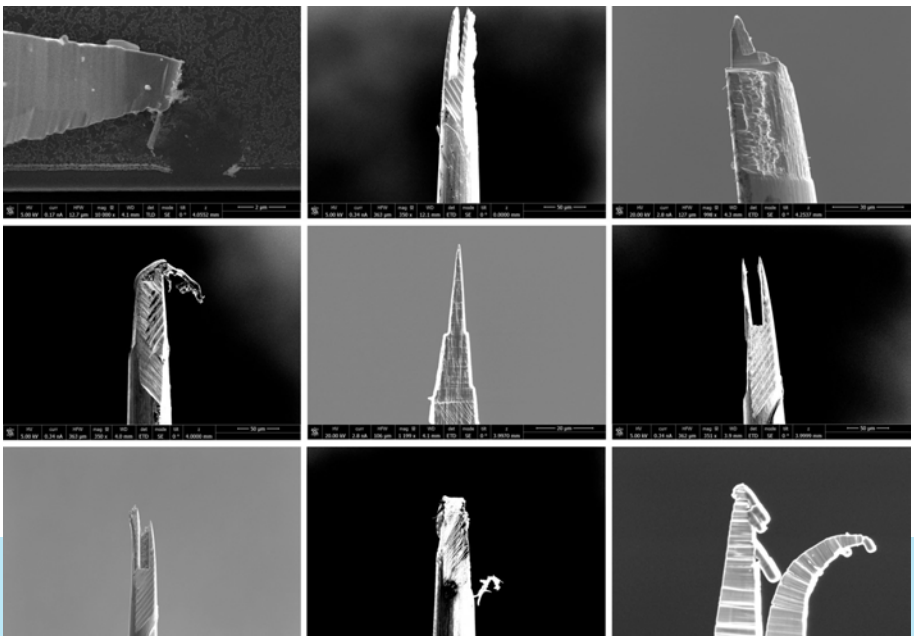
3. Scientific results

3.1. Publications

1. Boaretto, N; Rana, M; Marcilla, R; Vilatela, JJ. *Revealing the Mechanism of Electrochemical Lithiation of Carbon Nanotube Fibers*. **ACS APPLIED ENERGY MATERIALS 3,** 8695-8705, 2020.
2. Rubio, S; Maca, RR; Ortiz, GF; Vicente, CP; Lavela, P; Etacheri, V; Tirado, JL. *Iron Oxide-Iron Sulfide Hybrid Nanosheets as High-Performance Conversion-Type Anodes for Sodium-Ion Batteries*. **ACS APPLIED ENERGY MATERIALS 3,** 10765-10775, 2020.
3. Feng, WL; Maca, RR; Etacheri, V. *High-Energy-Density Sodium-Ion Hybrid Capacitors Enabled by Interface-Engineered Hierarchical TiO2 Nanosheet Anodes*. **ACS APPLIED MATERIALS & INTERFACES 12,** 4443-4453, 2020.
4. Fresta, E; Dosso, J; Cabanillas-Gonzalez, J; Bonifazi, D; Costa, RD. *Revealing the Impact of Heat Generation Using Nanographene-Based Light-Emitting Electrochemical Cells*. **ACS APPLIED MATERIALS & INTERFACES 12,** 28426-28434, 2020.
5. Pastrana, J; Dsouza, H; Cao, YQ; Figueroa, J; Gonzalez, I; Vilatela, JJ; Sepulveda, N. *Electrode Effects on Flexible and Robust Polypropylene Ferroelectret Devices for Fully Integrated Energy Harvesters*. **ACS APPLIED MATERIALS & INTERFACES 12,** 22815-22824, 2020.
6. Wen, WQ; Shuttleworth, PS; Yue, HB; Fernandez-Blazquez, JP; Guo, JW. *Exceptionally Stable Microporous Organic Frameworks with Rigid Building Units for Efficient Small Gas Adsorption and Separation*. **ACS APPLIED MATERIALS & INTERFACES 12,** 7548-7556, 2020.
7. Wang, Q; Su, DS; Wang, DY. *Carbon Nanotube/Epoxy Composites for Improved Fire Safety*. **ACS APPLIED NANO MATERIALS 3,** 4253-4264, 2020.
8. Elsaidi, SK; Ongari, D; Mohamed, MH; Xu, WQ; Motkuri, RK; Haranczyk, M; Thallapally, PK. *Metal Organic Frameworks for Xenon Storage Applications*. **ACS MATERIALS LETTERS 2,** 233-238, 2020.
9. Sonkusare, VN; Chaudhary, RG; Bhusari, GS; Mondal, A; Potbhare, AK; Mishra, RK; Juneja, HD; Abdala, AA. *Mesoporous Octahedron-Shaped Tricobalt Tetroxide Nanoparticles for Photocatalytic Degradation of Toxic Dyes*. **ACS OMEGA 5,** 7823-7835, 2020.
10. Zhang, J; Li, Z; Zhang, L; Yang, YX; Wang, DY. *Green Synthesis of Biomass Phytic Acid-Functionalized UiO-66-NH2 Hierarchical Hybrids toward Fire Safety of Epoxy Resin*. **ACS SUSTAINABLE CHEMISTRY & ENGINEERING 8,** 994-1003, 2020.
11. Alizadeh, R; LLorca, J. *Interactions between basal dislocations and beta(1)' precipitates in Mg-4Zn alloy: Mechanisms and strengthening*. **ACTA MATERIALIA 186,** 475-486, 2020.
12. Bellon, B; Haouala, S; LLorca, J. *An analysis of the influence of the precipitate type on the mechanical behavior of Al - Cu alloys by means of micropillar compression tests*. **ACTA MATERIALIA 194,** 207-223, 2020.

13. Esteban-Manzanares, G; Santos-Guemes, R; Papadimitriou, I; Martinez, E; LLorca, J. *Influence of the stress state on the cross-slip free energy barrier in Al: An atomistic investigation*. **ACTA MATERIALIA 184,** 109-119, 2020.
14. Liu, FY; Xin, RL; Zhang, MX; Perez-Prado, MT; Liu, Q. *Evaluating the orientation relationship of prismatic precipitates generated by detwinning in Mg alloys*. **ACTA MATERIALIA 195,** 263-273, 2020.
15. Liu, S; Martinez, E; LLorca, J. *Prediction of the Al-rich part of the Al-Cu phase diagram using cluster expansion and statistical mechanics*. **ACTA MATERIALIA 195,** 317-326, 2020.
16. Santos-Guemes, R; Bellon, B; Esteban-Manzanares, G; Segurado, J; Capolungo, L; LLorca, J. *Multiscale modelling of precipitation hardening in Al-Cu alloys: Dislocation dynamics simulations and experimental validation*. **ACTA MATERIALIA 188,** 475-485, 2020.
17. Wang, CY; Cepeda-Jimenez, CM; Perez-Prado, MT. *Dislocation-particle interactions in magnesium alloys*. **ACTA MATERIALIA 194,** 190-206, 2020.
18. Wang, JY; Molina-Aldareguia, JM; LLorca, J. *Effect of Al content on the critical resolved shear stress for twin nucleation and growth in Mg alloys*. **ACTA MATERIALIA 188,** 215-227, 2020.
19. Requena, G; Bugelnig, K; Sket, F; Milenkovic, S; Rodler, G; Weisheit, A; Gussone, J; Haubrich, J; Barriobero-Vila, P; Pusztai, T; Granasy, L; Theofilatos, A; da Silva, JC; Hecht, U. *Ultrafine Fe-Fe2Ti eutectics by directed energy deposition: Insights into microstructure formation based on experimental techniques and phase field modelling*. **ADDITIVE MANUFACTURING 33,** 101133, 2020.
20. Duan, YY; Ezquerro, C; Serrano, E; Lalinde, E; Garcia-Martinez, J; Berenguer, JR; Costa, RD. *Meeting High Stability and Efficiency in Hybrid Light-Emitting Diodes Based on SiO2/ZrO(2)Coated CsPbBr(3)Perovskite Nanocrystals*. **ADVANCED FUNCTIONAL MATERIALS 30,** 2005401, 2020.
21. Fresta, E; Costa, RD. *Advances and Challenges in White Light-Emitting Electrochemical Cells*. **ADVANCED FUNCTIONAL MATERIALS 30,** 1908176, 2020.
22. Fresta, E; Dosso, J; Cabanillas-Gonzalez, J; Bonifazi, D; Costa, RD. *Origin of the Exclusive Ternary Electroluminescent Behavior of BN-Doped Nanographenes in Efficient Single-Component White Light-Emitting Electrochemical Cells*. **ADVANCED FUNCTIONAL MATERIALS 30,** 1906830, 2020.
23. Fresta, E; Monclus, MA; Bertz, M; Ezquerro, C; Molina-Aldareguia, JM; Berenguer, JR; Kunimoto, M; Homma, T; Costa, RD. *Key Ionic Electrolytes for Highly Self-Stable Light-Emitting Electrochemical Cells Based on Ir(III) Complexes*. **ADVANCED OPTICAL MATERIALS 8,** 2000295, 2020.
24. Mahoro, GU; Fernandez-Cestau, J; Renaud, JL; Coto, PB; Costa, RD; Gaillard, S. *Recent Advances in Solid-State Lighting Devices Using Transition Metal Complexes Exhibiting Thermally Activated Delayed Fluorescent Emission Mechanism*. **ADVANCED OPTICAL MATERIALS 8,** 2000260, 2020.

25. Culebras, M; Ren, G; O'Connell, S; Vilatela, JJ; Collins, MN. *Lignin Doped Carbon Nanotube Yarns for Improved Thermoelectric Efficiency*. **ADVANCED SUSTAINABLE SYSTEMS 4,** 2000147, 2020.
26. Moya, A; Barawi, M; Aleman, B; Zeller, P; Amati, M; Monreal-Bernal, A; Gregoratti, L; O'Shea, VADP; Vilatela, JJ. *Interfacial studies in CNT fibre/TiO2 photoelectrodes for efficient H-2 production*. **APPLIED CATALYSIS B-ENVIRONMENTAL 268,** 118613, 2020.
27. Gussone, J; Bugelnig, K; Barriobero-Vila, P; da Silva, JC; Hecht, U; Dresbach, C; Sket, F; Cloetens, P; Stark, A; Schell, N; Haubrich, J; Requena, G. *Ultrafine eutectic Ti-Fe-based alloys processed by additive manufacturing - A new candidate for high temperature applications*. **APPLIED MATERIALS TODAY 20,** 100767, 2020.
28. Yusuf, A; Avvaru, VS; Dirican, M; Sun, CC; Wang, DY. *Low heat yielding electrospun phosphenanthrene oxide loaded polyacrylonitrile composite separators for safer high energy density lithium-ion batteries*. **APPLIED MATERIALS TODAY 20,** 100675, 2020.
29. Lilli, M; Sarasini, F; Di Fausto, L; Gonzalez, C; Fernandez, A; Lopes, CS; Tirillo, J. *Chemical Regeneration of Thermally Conditioned Basalt Fibres*. **APPLIED SCIENCES-BASEL 10,** 6674, 2020.
30. Martinez-Hergueta, F; Pellegrino, A; Ridruejo, A; Petrinic, N; Gonzalez, C; LLorca, J. *Dynamic Tensile Testing of Needle-Punched Nonwoven Fabrics*. **APPLIED SCIENCES-BASEL 10,** 5081, 2020.
31. Vila, M; Rubio-Zuazo, J; Lucas, I; Magen, C; Prados, A; Salas-Colera, E; Arnay, I; Castro, GR. *Ferromagnetic epitaxial Cr2O3 thin films grown on oxide substrates by Pulsed Laser Deposition*. **APPLIED SURFACE SCIENCE 534,** 147638, 2020.
32. Wang, ZJ; Liu, S; Qiu, ZX; Sun, HY; Liu, WC. *First-principles calculations on the interface of the Al/TiC aluminum matrix composites*. **APPLIED SURFACE SCIENCE 505,** 144502, 2020.
33. Wang, N; Liu, H; Zhang, J; Zhang, M; Fang, QH; Wang, DY. *Synergistic effect of graphene oxide and boron-nitrogen structure on flame retardancy of natural rubber/IFR composites*. **ARABIAN JOURNAL OF CHEMISTRY 13,** 6274-6284, 2020.



34. Caballero, FF; Ballesteros, JM; Garcia-Esquinas, E; Struijk, EA; Ortola, R; Rodriguez-Artalejo, F; Lopez-Garcia, E. *Are legume-based recipes an appropriate source of nutrients for healthy ageing? A prospective cohort study*. **BRITISH JOURNAL OF NUTRITION 124,** 943-951, 2020.
35. Cordani, M; Strippoli, R; Somoza, A. *Nanomaterials as Inhibitors of Epithelial Mesenchymal Transition in Cancer Treatment*. **CANCERS 12,** 25, 2020.
36. Salavagione, HJ; Shuttleworth, PS; Fernandez-Blazquez, JP; Ellis, GJ; Gomez-Fatou, MA. *Scalable graphene-based nanocomposite coatings for flexible and washable conductive textiles*. **CARBON 167,** 495-503, 2020.
37. Sanchez, JS; Maca, RR; Pendashteh, A; Etacheri, V; O'Shea, VAD; Castillo-Rodriguez, M; Palma, J; Marcilla, R. *Hierarchical Co3O4 nanorods anchored on nitrogen doped reduced graphene oxide: a highly efficient bifunctional electrocatalyst for rechargeable Zn-air batteries*. **CATALYSIS SCIENCE & TECHNOLOGY 10,** 1444-1457, 2020.
38. Maca, RR; Juarez, DC; Rodriguez, MC; Etacheri, V. *Nanointerface-driven pseudocapacitance tuning of TiO2 nanosheet anodes for high-rate, ultralong-life and enhanced capacity sodium-ion batteries*. **CHEMICAL ENGINEERING JOURNAL 391,** 123598, 2020.
39. Wang, Y; Vazquez-Rodriguez, I; Santos, C; Garcia-Quismondo, E; Palma, J; Anderson, MA; Lado, JJ. *Graphite felt 3D framework composites as an easy to scale capacitive deionization electrode for brackish water desalination*. **CHEMICAL ENGINEERING JOURNAL 392,** 123698, 2020.
40. Zhang, J; Li, Z; Shao, ZB; Zhang, L; Wang, DY. *Hierarchically tailored hybrids via interfacial-engineering of self-assembled UiO-66 and prussian blue analogue: Novel strategy to impart epoxy high-efficient fire retardancy and smoke suppression*. **CHEMICAL ENGINEERING JOURNAL 400,** 125942, 2020.
41. Zhang, ZD; Han, ZQ; Pan, YT; Li, DH; Wang, DY; Yang, RJ. *Dry synthesis of mesoporous nanosheet assembly constructed by cyclomatrix polyphosphazene frameworks and its application in flame retardant polypropylene*. **CHEMICAL ENGINEERING JOURNAL 395,** 125076, 2020.
42. Zhang, ZD; Qin, JY; Zhang, WC; Pan, YT; Wang, DY; Yang, RJ. *Synthesis of a novel dual layered double hydroxide hybrid nanomaterial and its application in epoxy nanocomposites*. **CHEMICAL ENGINEERING JOURNAL 381,** 122777, 2020.
43. Pan, YT; Yuan, YS; Wang, DY; Yang, RJ. *An Overview of the Flame Retardants for Poly(vinyl chloride): Recent States and Perspective(dagger)*. **CHINESE JOURNAL OF CHEMISTRY 38,** 1870-1896, 2020.
44. Sebaey, TA; Catalanotti, G; Lopes, CS; O'Dowd, N. *Computational micromechanics of the effect of fibre misalignment on the longitudinal compression and shear properties of UD fibre-reinforced plastics*. **COMPOSITE STRUCTURES 248,** 112487, 2020.
45. Li, YM; Hu, SL; Wang, DY. *Polymer-based ceramifiable composites for flame retardant applications: A review*. **COMPOSITES COMMUNICATIONS 21,** 100405, 2020.

46. Bergan, AC; Herraez, M; Gonzalez, C; Lopes, CS. *A constitutive model for fiber kinking: Formulation, finite element implementation, and verification*. **COMPOSITES PART A-APPLIED SCIENCE AND MANUFACTURING 129,** 105682, 2020.
47. Herraez, M; Segurado, J; Gonzalez, C; Lopes, CS. *A microstructures generation tool for virtual ply property screening of hybrid composites with high volume fractions of non-circular fibers - VIPER*. **COMPOSITES PART A-APPLIED SCIENCE AND MANUFACTURING 129,** 105691, 2020.
48. Zhang, L; Liu, W; Wen, X; Chen, JY; Zhao, CS; Castillo-Rodriguez, M; Yang, LW; Zhang, XQ; Wang, R; Wang, DY. *Electrospun submicron NiO fibers combined with nanosized carbon black as reinforcement for multi-functional poly(lactic acid) composites*. **COMPOSITES PART A-APPLIED SCIENCE AND MANUFACTURING 129,** 105662, 2020.
49. Ou, YF; Gonzalez, C; Vilatela, JJ. *Understanding interlaminar toughening of unidirectional CFRP laminates with carbon nanotube veils*. **COMPOSITES PART B-ENGINEERING 201,** 108372, 2020.
50. Pascual-Gonzalez, C; Iragi, M; Fernandez, A; Fernandez-Blazquez, JP; Aretxabaleta, L; Lopes, CS. *An approach to analyse the factors behind the micromechanical response of 3D-printed composites*. **COMPOSITES PART B-ENGINEERING 186,** 107820, 2020.
51. Zhang, J; Li, Z; Qi, XL; Zhang, W; Wang, DY. *Size tailored bimetallic metal-organic framework (MOF) on graphene oxide with sandwich-like structure as functional nano-hybrids for improving fire safety of epoxy*. **COMPOSITES PART B-ENGINEERING 188,** 107881, 2020.
52. Castro, J; Sket, F; Gonzalez, C. *S-XCT experimental determination of local contact angle and meniscus shape in liquid moulding of composites*. **COMPOSITES SCIENCE AND TECHNOLOGY 199,** 108362, 2020.
53. Wen, X; Liu, ZQ; Li, Z; Zhang, J; Wang, DY; Szymanska, K; Chen, XC; Mijowska, E; Tang, T. *Constructing multifunctional nanofiller with reactive interface in PLA/CB-g-DOPO composites for simultaneously improving flame retardancy, electrical conductivity and mechanical properties*. **COMPOSITES SCIENCE AND TECHNOLOGY 188,** 107988, 2020.
54. Portillo, D; Oesterle, B; Thierer, R; Bischoff, M; Romero, I. *Structural models based on 3D constitutive laws: Variational structure and numerical solution*. **COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING 362,** 112872, 2020.
55. Garcia, IG; Haranczyk, M. *Toward crystalline porosity estimators for porous molecules*. **CRYSTENGCOMM 22,** 7242-7251, 2020.
56. Xiao, Y; Guo, BB; Zhang, J; Hu, C; Ma, RG; Wang, DY; Wang, JC. *A bimetallic MOF@graphene oxide composite as an efficient bifunctional oxygen electrocatalyst for rechargeable Zn-air batteries*. **DALTON TRANSACTIONS 49,** 5730-5735, 2020.
57. Wang, Q; Zhang, J; Shi, W; Castillo-Rodriguez, M; Su, DS; Wang, DY. *Coordinating mechanical performance and fire safety of epoxy resin via functionalized nanodiamond*. **DIAMOND AND RELATED MATERIALS 108,** 107964, 2020.

58. Santos, C; Garcia-Quismondo, E; Palma, J; Anderson, MA; Lado, JJ. *Understanding capacitive deionization performance by comparing its electrical response with an electrochemical supercapacitor: Strategies to boost round-trip efficiency*. **ELECTROCHIMICA ACTA 330,** 135216, 2020.
59. Zhang, L; Li, Z; Wang, DY. *Polydopamine-assisted strategies for preparation of fire-safe polymeric materials: A review*. **EUROPEAN POLYMER JOURNAL 138,** 109973, 2020.
60. Yang, YX; Haurie, L; Zhang, J; Zhang, XQ; Wang, R; Wang, DY. *Effect of bio-based phytate (PA-THAM) on the flame retardant and mechanical properties of polylactide (PLA)*. **EXPRESS POLYMER LETTERS 14,** 705-716, 2020.
61. Rueda-Ruiz, M; Monclus, MA; Beake, B; Galvez, F; Molina-Aldareguia, JM. *High strain rate compression of epoxy micropillars*. **EXTREME MECHANICS LETTERS 40,** 100905, 2020.
62. Yang, LW; Mayer, CR; Chawla, N; LLorca, J; Molina-Aldareguia, JM. *Nanomechanical characterization of the fracture toughness of Al/SiC nanolaminates*. **EXTREME MECHANICS LETTERS 40,** 100945, 2020.
63. Pan, YT; Wang, DY. *Functionalized Layered Nanomaterials towards Flame Retardant Polymer Nanocomposites*. **FLAME RETARDANT POLYMERIC MATERIALS: A HANDBOOK ,** 181-212, 2020.
64. Corzo-Martinez, M; Banares, C; Diaz, A; Vazquez, L; Reglero, G; Torres, CF. *In vitro digestibility and bioaccessibility of lipid-based delivery systems obtained via enzymatic glycerolysis: a case study of rosemary extract bioaccessibility*. **FOOD & FUNCTION 11,** 813-823, 2020.
65. Yue, HB; Zheng, YR; Zheng, PX; Guo, JW; Fernandez-Blazquez, JP; Clark, JH; Cui, YD. *On the improvement of properties of bioplastic composites derived from wasted cottonseed protein by rational cross-linking and natural fiber reinforcement*. **GREEN CHEMISTRY 22,** 8642-8655, 2020.
66. Alvaredo-Atienza, A; Fernandez-Blazquez, JP; Castell, P; de Villoria, RG. *Production of graphene nanoplate/polyetheretherketone composites by semi-industrial melt-compounding*. **HELIYON 6,** e03740, 2020.
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68. Isensee, T; Tourret, D. *Three-dimensional needle network model for dendritic growth with fluid flow*. **INTERNATIONAL CONFERENCE ON MODELLING OF CASTING, WELDING AND ADVANCED SOLIDIFICATION PROCESSES (MCWASP XV) 861,** 12049, 2020.
69. Tourret, D; Sturz, L; Viardin, A; Zaloznik, M. *Comparing mesoscopic models for dendritic growth*. **INTERNATIONAL CONFERENCE ON MODELLING OF CASTING, WELDING AND ADVANCED SOLIDIFICATION PROCESSES (MCWASP XV) 861,** 12002, 2020.
70. Lucarini, S; Segurado, J. *An upscaling approach for micromechanics based fatigue: from RVEs to specimens and component life prediction*. **INTERNATIONAL JOURNAL OF FRACTURE 223,** 93-108, 2020.

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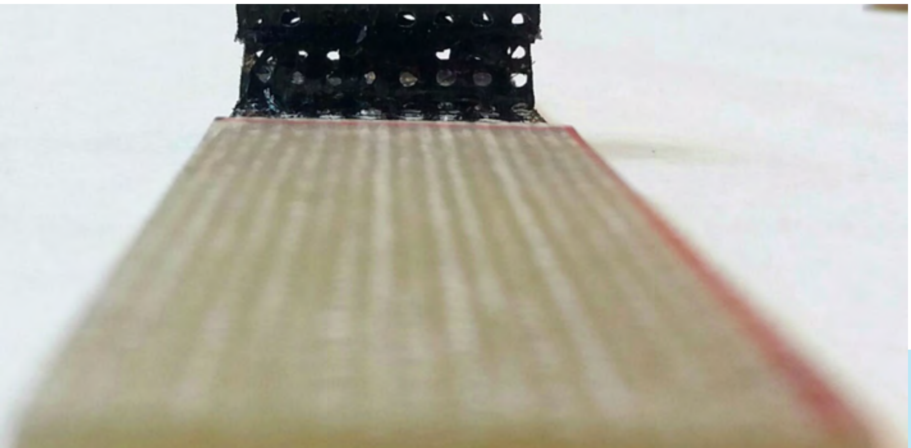

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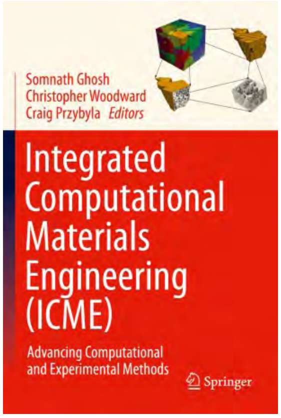
3.2. Book chapters

1. A. Cruzado, J. Llorca, J. Segurado . *Computational Micromechanics Modeling of Polycrystalline Superalloys: Application to Inconel 718*. In **Integrated Computational Materials Engineering (ICME): Advancing Computational and Experimental Methods, Springer**, 127-163, 2020.
2. M. Rana, C. Santos, A. Monreal-Bernal, J. J. Vilatela. *Synthesis, Characterization, and Applications in Energy Management.* In **Synthesis and Applications of Nanocarbons, Wiley,** 2020.
3. V. S. Avvaru, M. Vincent, V. Etacheri. *Advanced Lithium- Ion Batteries for Electric Vehicles: Promise and Challenges of Nanostructured Electrode Materials*. In **Rechargeable Lithium-Ion Batteries Trends and Progress in Electric Vehicles**, **CRC press**, 2020.



3.3. Patent applications

1. *Electrode comprising oxygen-deficient rutile TiO_2 nanowires and uses thereof*. IMDEA Materials Institute. Patent application number EP20382542.7 (22 June 2020)
2. *A method for the large scale synthesis of metal oxide nanosheets, and their uses*. IMDEA Materials Institute. Patent application number EP20383049.2 (2 December 2020)

3.4. Software registered

1. *MULTIFOAM*. IMDEA Materials Institute and Technical University of Madrid. Registro Territorial de la Propiedad Intelectual, Comunidad de Madrid (28 February 2020).

3.5. International Conferences

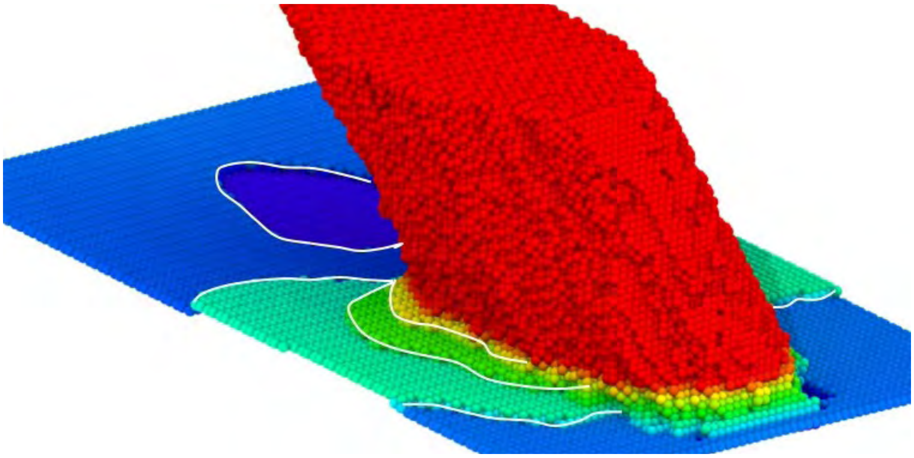
Invited and plenary talks

1. *"The use of diffusion couples and micropillar compression to determine alloying effects on the CRSS for slip and twinning in Mg alloys"*, J. M. Molina-Aldarequia, **4th Schöntal Symposium 2020 on "Dislocation-based Plasticity**, Schöntal, Germany, March 2020
2. *"Comparing mesoscopic models for dendritic growth"*, D. Tourret, **MCWASP: Modelling of Casting, Welding and Advanced Solidification Processes**, virtual event, June 2020.
3. *"Co3O4 decorated TiO2 nanosheets as highly pseudocapacitive cathodes for long lasting rechargeable Mg-Li hybrid batteries"*, M. Vincent, **International Conference on Nanomaterials Science and Mechanical Engineering**, virtual event, Portugal, June 2020.
4. *"Rapid response: qualification and certification during a crisis"*, M.T. Pérez-Prado **4th ASTM Additive Manufacturing Center of Excellence Snapshot Workshop**, virtual event, September 2020.
5. *"Research activities of the Powder Metallurgy Group (GTP) at UC3M and IMDEA Materials Institute using Field Assisted Sintering Techniques"*, J. M. Torralba, **III National Workshop on Spark Plasma Sintering**, Krakov, Poland, October 2020.
6. *"High-Entropy Alloys and high temperature applications: an opportunity for PM"*, J. M. Torralba, **EUROPM2020**, virtual event, October 2020.
7. *"Coupling micro and mesostructure in Inconel 3D printed lattices"*, S. Banait, **Virtual Workshop on "AM related to aerospace"/UK Forum for Structural Integrity**, virtual event, November 2020.
8. *"Modeling of polycrystalline solidification from dendrites to grain microstructures"*, D. Tourret, **COMPSAFE: International Conference on Computational Engineering and Science for Safety and Environmental Problems**, virtual event, December 2020.

Regular contributions

1. *"Pseudocapacitance driven ultralong life Mg-Li hybrid batteries based on TiO2 nanosheet cathodes"*, M. Vincent, V. Etacheri, **National seminar on current trends in chemistry (CTriC2020)**, Cochin, India, February 2020.
2. *"High-throughput discovery of metal-organic frameworks for cooperative CO2 adsorption"*, E. Taw, J. R. Long, J. B. Neaton, M. Haranczyk, **APS March Meeting 2020**, Denver, USA, March 2020.
3. *"Manufacturability of Inconel 718 lattices structures by selective laser melting"*, S. Banait, M. Campos, M. T. Pérez-Prado, **23rd International Conference on Materials Forming (ESAFORM 2020)**, virtual event, May 2020.

4. *"Ultralong-life Mg-Li hybrid batteries based of pseudocapacitive Co3O4-TiO2 hybrid nanosheet cathodes"*, M. Vincent, V. Etacheri, **International virtual conference: Electric mobility 2020**, virtual event, June 2020.
5. *"Three-dimensional needle network model for dendritic growth with fluid flow",* T. Isensee, D. Tourret, **MCWASP: Modelling of Casting, Welding and Advanced Solidification Processes,** virtual event, June 2020.
6. *"Accelerating development of natural porous materials assisted by statistical machine learning"*, G. Lo Dico, V. Carcelen, M. Haranczyk, **International Conference on Machine Learning**, Siena, Italy, July 2020.
7. *"Pseudocapacitive hybrid TiO2 cathode for long-lasting Mg-Li dual ion batteries"*, M. Vincent, V. Etacheri, **Virtual international transdisciplinary conference**, virtual event, August 2020.
8. *"Accelerating development of natural porous materials assisted by statistical machine learning"*, G. Lo Dico, V. Carcelen, M. Haranczyk, **Chemical Science Symposium 2020: How can machine learning and autonomy accelerate chemistry?**, virtual event, September 2020.
9. *"Long-lasting Mg-Li hybrid batteries based on pseudocapacitive TiO2 nanosheet cathodes"*, M. Vincent, V. Etacheri, **14th International Conference on Surfaces, Coatings and Nanostructured Materials** , London, UK, September 2020.
10. *"High Entropy Alloys, A New Opportunity For The Powder Metallurgy Route"*, J. M. Torralba, P. Alvaredo, A. García-Junceda, **EUROPM2020**, virtual event , October 2020.
11. *"Lattice Distortion Study In Co-based Superalloys Produced By PM Route With Low W Content"*, J. M. Torralba, H. Sanz-Nicolas, M. Campos, M. Cartón-Cordero, S-J. Hong, **EUROPM2020**, virtual event, October 2020.



12. *"Effect of oxygen vacancies on the electrochemical performance of Anatase TiO2 as Mg-Li hybrid battery cathode"*, M. Vincent, V. Etacheri, **9th Symposium on Electrochemistry in Nanoscience**, Paris, France, November 2020.
13. *"Interface engineered CoO@3D-NRGO pseudocapacitive anodes for high energy/ power density lithium-ion batteries"*, V. S. Avvaru, V. Etacheri, **9th Symposium on Electrochemistry in Nanoscience**, Paris, France, November 2020.
14. *"Nanointerface-Driven Pseudocapacitance Tuning of TiO2 Anode for Sodium-Ion Batteries"*, R. R. Maca, V. Etacheri, **9th Symposium on Electrochemistry in Nanoscience**, Paris, France, November 2020.

Membership in organising committees

1. **School and industry day on 3D printing of metals**, M. T. Pérez-Prado (Organizer), Madrid, Spain, January 2020.
2. **2020 International Symposium on Flame-Retardant Materials (ISFRMT2020)**, D-Y Wang (Member of the Scientific Committee), Qingdao, China, September 2020.
3. **EUROPM2020**, J. M. Torralba (Member of the Technical Programme Committee), virtual event, October 2020.
4. **COMPSAFE: International Conference on Computational Engineering and Science for Safety and Environmental Problems**, D. Tourret (Symposium Organiser), virtual event, December 2020.

3.6. Invited seminars and lectures

1. *"Computational modeling of metal additive manufacturing: Recent advances and outstanding challenge",* D. Tourret, **MAT4.0 Winter School on 3D printing of Metals**, Madrid, Spain, January 2020.
2. *"Science and applications of CNT fibres and related macromolecular materials*", J. J. Vilatela, **Trinity College Dublin**, Dublin, UK, January 2020
3. *"Microstructure sensitive fatigue in polycrystalline superalloys: from micromechanics to specimen life prediction*", J. Segurado, **Solid Mechanics Laboratory (LMS), Ecole Polytechnique**, Paris, France, February 2020.
4. *"High-throughput experimental techniques to measure the CRSS for slip and twinning in Mg and Mg alloys""*, J. Llorca, **Sharif University of Technology**, Tehran, Iran, April 2020.
5. *"3D printing of metals*", M. T. Pérez Prado, **University of Prince Edward Island**, Charlottetown, Canada, June 2020.
6. *"Semiconductor photocatalysis: Advances and applications*", V. Etacheri, **Mar Ivanios College, Kerala University**, Kerala, India, June 2020.
7. *"PM Production Routes*", J. M. Torralba, **European Powder Metallurgy Association, Young Engineers Day**, virtual event, September 2020

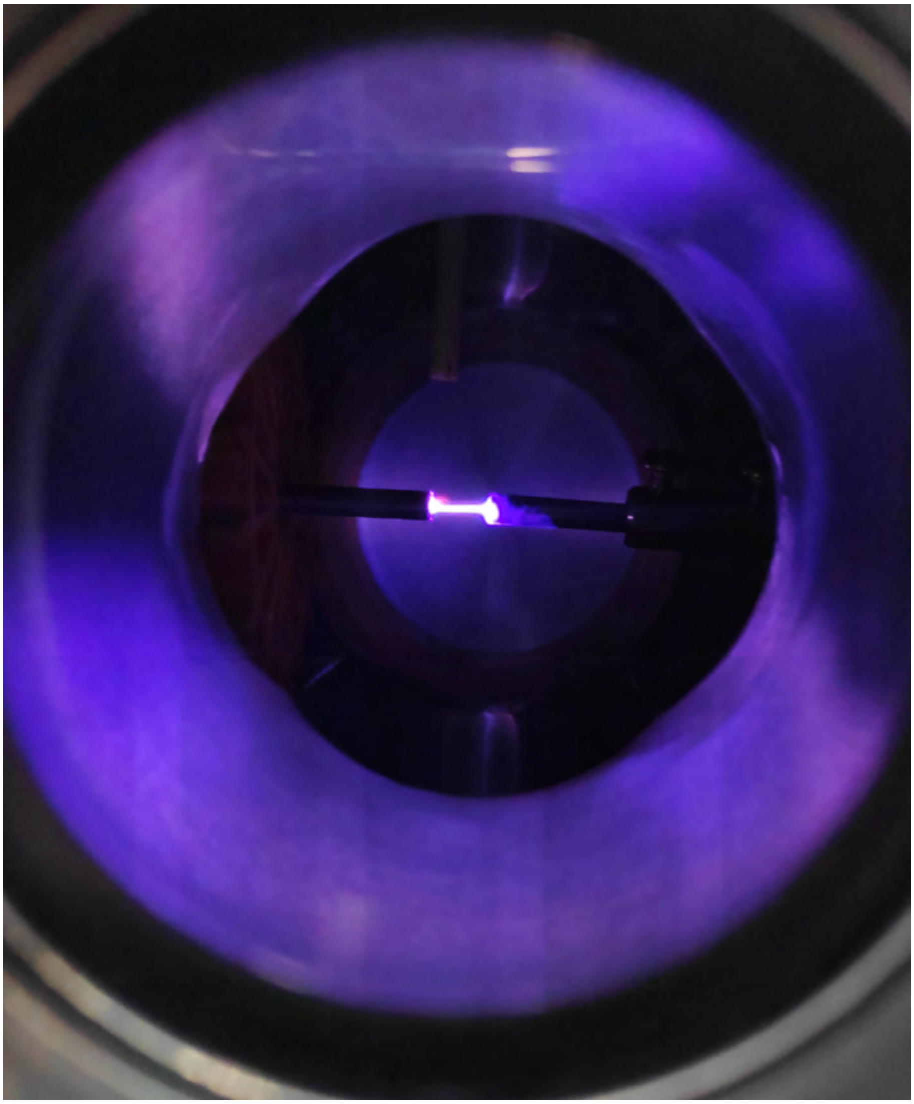
8. *"CNT fibres and their polymer composites: open questions and recent industrialisation efforts*", J. J. Vilatela, **University of Manchester**, Manchester, UK, September 2020.
9. *"Dislocation-particle interactions in Mg alloys*", M. T. Pérez Prado, **Indian Institute of Science**, Bangalore, India, September 2020.
10. *"Investigación e innovación en materiales avanzados con aplicación al sector ferroviario*", J.J. Vilatela, **Jornada MATERPLAT sobre "Investigación e innovación en materiales avanzados con aplicación al sector ferroviario"**, Madrid, Spain, October 2020.
11. *"Fundamentals of Press and Sintering*", J. M. Torralba, **European Powder Metallurgy Association, Webinar on Press and Sintering**, virtual event, November 2020.
12. *"Microstructure formation during solidification processes: Theory & modeling across scales",* D. Tourret, **Guangdong Technion-Israel Institute of Technology**, virtual event, December 2020.
13. *"Virtual Testing of Structural Composites: a multiscale perspective.*", C. González, **3rd OptiMACS Network Short Course**, virtual event, December 2020
14. *"Nex generation rechargeable batteries through defect engineering*", V. Etacheri, **Kannur University**, Kerala, India, December 2020.

3.7. Awards

1. Best PdD thesis 2020, Technical University of Madrid, **A. Monreal.**
2. TMS Young Leader Professional Development Award, The Minerals, Metals & Materials Society (TMS), **D. Tourret.**
3. Outstanding Reviewer Award 2019, Acta & Scripta Materialia, **D. Tourret.**
4. Outstanding Key Reader Award 2019, Metallurgical & materials Transactions A, **D. Tourret.**
5. Outstanding presentation at the "Chemical Science Symposium 2020: How can machine learning and autonomy accelerate chemistry", Royal Society of Chemistry (RSC), **G. Lo Dico.**
6. Best PhD thesis, Technical University of Madrid, **J. Wang.**
7. Best PdD thesis 2020, Technical University of Madrid, **J. C. Fernández.**
8. Brahm Prakash Chair Professorship 2020-2021, Indian Institute of Science, **M.T. Pérez-Prado.**
9. Numerary Member of the Academia Joven de España, Academia Joven de España, **R. D. Costa.**
10. FPdGi research award by the Spanish Royal Family, Fundacion Princesa de Girona, **R. D. Costa.**
11. Fellow of the Royal Society of Chemistry, Royal Society of Chemistry, **R. D. Costa.**

3.8. Seminars

1. *"Next Generation Biomaterials for Health Care"* **Dr. Jennifer Patterson** (from BIOFABICS in Portugal). January 2020.
2. *"Development of Biodegradable Magnesium-Based Supports for Stem Cell Therapy of Vascular Disease"* **Dr. Monica Echeverry** (from the University of Shaghai Jiao Tong). January 2020
3. *"Twin transmission across grain boundaries in Mg"* **Dr. Laurent Capolungo** (from Los Alamos National Laboratory). March 2020.



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 our technological offer ready to be transferred to industry, other research institutions, investors or entrepreneurs.

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

Title: Energy storage in multifunctional structural composite material
Description: Laminar composite material simultaneously having excellent structural properties and high energy storage efficiency.
Opportunity: Technology license

Title: Ultrafast charging Li-ion batteries based on nanostructured electrodes
Description: High capacity nanostructured anodes (1D and 2D morphologies) for ultrafast-charging Li-ion batteries.
Opportunity: Technology license

Title: Ultralong life Mg batteries based on engineered cathodes
Description: Cathodes of high capacity and ultralong life for Mg batteries.
Opportunity: Technology license

Title: VIPER (VIrtual Ply propERty)
Description: 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

Title: Electrode for capacitive deionization
Description: 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

Title: Multifunctional sensor for composite materials
Description: 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

Title: FFTMAD (Fast Fourier Transform based homogenization code, MADrid)
Description: 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

Title: Resistive curing of polymers and composite materials
Description: 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

Title: MULTIFOAM
Description: 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

Title: IRIS
Description: 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

Title: MUESLI
Description: 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

Title: CAPSUL
Description: CAPSUL is a package of crystal plasticity and polycrystalline homogenization simulation tools.
Opportunity: Software license

Title: A halogen free flame retardant epoxy resin composition
Description: New halogen free flame retardant epoxy resin with excellent mechanical properties, thermal resistance, low smoke release and good processability, which can also be used as adhesive.
Opportunity: Technology license

5. Training, communication and outreach

5.1. Theses

PhD Theses

1. *"Development and characterization of advanced thin coatings on nanostructured titanium for biomedical applications"*
   Student: Hugo Mora
   Carlos III University of Madrid
   Advisor: Dr. I.Sabirov; Prof. E. Matykina and Dr. J. M. Molina-Aldareguia
   Date of defense: February 2020

2. *"Microstructural design via ultrafast heating to improve mechanical properties of a low carbon steel"*
   Student: Miguel A. Valdés
   Carlos III University of Madrid
   Advisor: Dr. I. Sabirov
   Date of defense: April 2020

3. *"High Strain Rate Mechanical Behavior of Advanced High Strength Steels"*
   Student: Peikang Xia
   Technical University of Madrid
   Advisor: Dr. I. Sabirov
   Date of defense: September 2020

4. *"Multiscale Experimental Characterization and Modelling Validation of Microstructure and Mechanical Properties of Engineering Alloys"*
   Student: Bárbara Bellón
   Technical University of Madrid
   Advisor: Prof. J. Llorca and Dr. I. Sabirov
   Date of defense: September 2020

5. *"Microstructure based fatigue simulation using Fast Fourier Transform based homogenization"*
   Student: Sergio Lucarini
   Technical University of Madrid
   Advisor: Prof. J. Segurado
   Date of defense: March 2020

6. *"Fatigue Growth Of Microstructurally Short Cracks In Ni-Based Superalloys"*
   Student: Marcos Jiménez
   Carlos III University of Madrid
   Advisor: Dr. J. M. Molina-Aldareguia
   Date of defense: June 2020

7. *"Development and characterization of advanced thin coatings on nanostructured titanium for biomedical applications"*
   Student: Hugo Mora
   Carlos III University of Madrid
   Advisor: Dr. I. Sabirov; Dr. J. M. Molina-Aldareguia and Dr. E. Matykina
   Date of defense: February 2020

8. *"Hybrid FRP/CNT veil hierarchical composites with enhanced interlaminar properties and integrated multifunctionalities"*
   Student: Yunfu Ou
   Technical University of Madrid
   Advisor: Prof. C. González
   Date of defense: November 2020

9. *"Filler surface functionalization for flame retardant epoxy composites"*
   Student: Lu Zhang
   Technical University of Madrid
   Advisor: Dr. D-Y Wang
   Date of defense: September 2020

10. *"Beyond traditional emitters in light-emitting electrochemical cells"*
    Student: Elisa Fresta
    Autonomous University of Madrid
    Advisor: Dr. R. Costa
    Date of defense: September 2020

11. *"BioHLEDs- fluorescent proteins as color down-converting filter"*
Student: Veronica Fernandez-Luna
Autonomous University of Madrid
Advisor: Dr. R. Costa
Date of defense: October 2020

12. *"Preliminary study on the industrial preparation of high- performance nanocarbon/ epoxy composites for vehicle body"*
Student: Qi Wang
Advisor: Dr. D-Y Wang
Date of defense: July 2020

Master/Bachelor Theses

1. *"Caracterización dinámica de materiales compuestos de epoxi reforzados con fibra de carbono"*
Student: Alexander Mejía
Carlos III University of Madrid
Advisor: Dr. J. M. Molina-Aldareguia
Date of defense: October 2020

2. *"Mecánica de fieltros nanoestructurados"*
Student: Carlos del Castillo
Technical University of Madrid
Advisor: Dr. Juan José Vilatela
Date of defense: October 2020

3. *"Optimization of a gas atomization system for additive manufacturing of gamma-TiAl"*
Student: Arturo Martín
Carlos III University of Madrid
Advisor: Dr. M.T. Pérez-Prado
Date of defense: July 2020

4. *"Dynamic mechanical characterization of carbon fiber reinforced composites"*
Student: Alexander Mejía
Carlos III University of Madrid
Advisor: Dr. F. Sket
Date of defense: October 2020

5. *"Use of ionic additives for the stabilization of fluorescent proteins in polymeric medium"*
Student: Jorge González
Complutense University of Madrid
Advisor: Dr. R. Costa
Date of defense: March 2020

6. *"Manufacturing of polymeric filaments for 3D printing of biodegradable scaffolds for biomedical applications"*
Student: Nicolás Biurrun
Technical University of Madrid
Advisor: Prof. J. Llorca and Dr. C. Pascual
Date of defense: September 2020

7. *"Análisis y control de la señal electrónica de máquinas universales de ensayo de materiales"*
Student: Pablo Martínez
Carlos III University of Madrid
Advisor: Dr. J. J. Vilatela
Date of defense: March 2020

8. *"Estudio sobre la generación y propagación de microgrietas en laminados en CFRP sometidos a cargas térmicas"*
Student: Javier Martínez
Technical University of Madrid
Advisor: Prof. C. González
Date of defense: October 2020

9. *"Fabricación, caracterización mecánica de materiales compuestos reforzados con interleaves de nanotubos, fractura interlaminar"*
Student: Jorge Naranjo
Technical University of Madrid
Advisor: Prof. C. González
Date of defense: October 2020

10. *"Procesamiento de aleaciones de TiAlNi por Compactación en Caliente Asistida por Campo Eléctrico (FAHP)"*
Student: Rafael Herrera
Carlos III University of Madrid
Advisor: Dr. I. Sabirov
Date of defense: October 2020

11. *“Simulation of tungsten mechanical behavior through crystal plasticity and FFT-based method”*
Student: Elena Botica
Technical University of Madrid
Advisor: Prof. J. Segurado
Date of defense: September 2020

12. *“Development and validation of a FFT framework for studying lattice materials”*
Student: Anthony Voitus
Technical University of Madrid
Advisor: Prof. J. Segurado
Date of defense: September 2020

13. *“Micromechanical study of ceramic matrix composites”*
Student: Jinxue Ding
Technical University of Madrid
Advisor: Dr. J. M. Molina-Aldareguia
Date of defense: January 2020

5.2. Internships / Visiting students

1. *“Using machine learning to accelerate the prediction of metallic microstructures”*
Student: Diego Muñoz
Advisor: Dr. D. Tourret
Visiting student from: Technical University of Madrid
Period: June 2020 - September 2020

2. *“A numerical model for shape memory alloys”*
Student: Diego Ruiz
Advisor: Dr. I. Romero
Visiting student from: InTalentia
Period: July 2020 - September 2020

3. *“Martensitic stainless steels via quenching and partitioning process”*
Student: Berta Ruiz
Advisor: Dr. I. Sabirov
Visiting student from: InTalentia
Period: June 2020 - August 2020

4. *“Fabricación aditiva de materiales biodegradables para aplicaciones biomédicas”*
Student: Sara Cameron
Advisor: Prof. J. Llorca
Visiting student from: InTalentia/Fundación Dádoris
Period: July 2020 - July 2020

5. *"Assessment of the effect of elastic strains on catalytic properties by means of atomistic simulations"*
Student: Carmen Martínez
Advisor: Prof. J. Llorca
Visiting student from: InTalentia
Period: September 2020 - October 2020

6. *"Development of machine learning algorithms to predict the processing-microstructure link during additive manufacturing"*
Student: Patricia Caño
Advisor: Dr. G. Esteban and C. Galera
Visiting student from: Technical University of Madrid
Period: October 2020 - April 2020

7. *"Multi-scale Optimisation for Additive Manufacturing of fatigue resistant shock-absorbing MetaMaterials"*
Student: Marcos Rodriguez
Advisor: Prof. J. Segurado
Visiting student from: Eindhoven University of Technology
Period: September 2020 - November 2020

8. *"Development and validation of a FFT framework for studying lattice materials"*
Student: Anthony Voitus
Advisor: Prof. J. Segurado
Visiting student from: Technical University of Madrid
Period: February 2020 - June 2020

9. *"Micromechanical characterization of ceramic matrix composites"*
Student: Jinxue Ding
Advisor: Dr. J. M. Molina-ALdareguia
Visiting student from: Technical University of Madrid
Period: June 2019 - January 2020

10. *"Internship Bachelor Degree - Mecnical Engineering"*
Student: José Colao
Advisor: Prof. J. M. Torralba and Dr. A. Páez
Visiting student from: Europea of Madrid University
Period: January 2020 - June 2020

11. *"Nanostructured batteries"*
Student: Quim Gispert
Advisor: Dr. J. J. Vilatela
Visiting student from: InTalentia/ Ramón Llull University
Period: August 2020 - November 2020

12. *"Market analysis of materials for new generation batteries"*
Student: Rishin Banerjee
Advisor: Dr. J. J. Vilatela and Dr. J. Rubio
Visiting student from: IESE
Period: June 2020 - August 2020

13. *"Piezoresistive properties of nanostructured networks"*
Student: Ángel Labordet
Advisor: Dr. J. J. Vilatela
Visiting student from: Carlos III University of Madrid
Period: September 2020 - December 2020

14. *"Microstructure and mechanical property analysis on the CNT fibers"*
Student: Junyeon Hwang
Advisor: Dr. J. J. Vilatela
Visiting student from: Korea Institute of Science & Technology (KIST)
Period: December 2019 - February 2020

15. *"Towards data-driven stability predictors for metal-organic framework materials"*
Student: Marta Chaves
Advisor: Dr. M. Haranczyk
Visiting student from: InTalentia
Period: July 2020 - September 2020

16. *"Procesado y caracterización in-situ de materiales"*
Student: Jonathan Espinoza
Advisor: Dr. F. Sket
Visiting student from: InTalentia
Period: July 2020 - November 2020

17. *"Dynamic behaviour of composite materials for next generation aeroengines "*
Student: Joaquín Bolado
Advisor: Dr. F. Sket
Visiting student from: Complutense University of Madrid
Period: October 2019 - August 2020

18. *"Development of novel bio-based phase change materials for thermal"*
Student: Alba Marta López
Advisor: Dr. D-Y Wang
Visiting student from: Technical University of Madrid
Period: October 2020 - March 2021

19. *"Development of Novel Flame retardant Polymer Electrolytes for Lithium-ion Batteries"*
Student: Sun Chanchung
Advisor: Dr. D-Y Wang
Visiting student from: Technical University of Madrid
Period: May 2019 - January 2020

20. *"Design and study new generation fire safety batteries for advanced application "*
Student: María Benito
Advisor: Dr. D-Y Wang
Visiting student from: InTalentia
Period: July 2020 - September 2020

21. *"Copper(I) complexes for light-emitting electrochemical cells"*
Student: Gilbert Mahoro
Advisor: Dr. R. Costa
Visiting student from: ENSICAEN
Period: October 2017 - August 2020

5.3. Teaching in Masters

1. *"Simulation"*
Master in Materials Engineering
Technical University of Madrid
Professor: Prof. C González

2. *"Design and manufacturing of Advanced Composite Materials"*
Master in Materials Engineering
Technical University of Madrid
Professor: Prof. C..González

3. *"Simulation in materials engineering"*
Master in Materials Engineering
Technical University of Madrid
Professor: Dr. D. Tourret

4. *"Structural Characterization of Materials II: Spectroscopy"*
Master in Materials Engineering
Technical University of Madrid
Professor: Dr. F. Sket

5. *"Advanced simulation methods"*
Master in Industrial Engineering
Technical University of Madrid
Professor: Prof. I. Romero

6. *"Metal Matrix Composites"*
Master in Composite Materials
Technical University of Madrid / AIRBUS
Professor: Dr. I. Sabirov

7. *"Simulation"*
Master in Materials Engineering
Technical University of Madrid
Professor: Prof. J. Segurado

8. *"Simulation in materials science and engineering"*
Master in Materials Science and Engineering
Carlos III University of Madrid
Professor: Dr. J. M. Molina-Aldareguia

9. *"Advanced Composite Materials"*
Master in Materials Science and Engineering

Carlos III University of Madrid
Professor: Dr. J. M. Molina-Aldareguia

10. *"Nanomaterials - Nanocarbons"*
Master in Materials Science and Engineering
Carlos III University of Madrid
Professor: Dr. J. J. Vilatela

11. *"Hierarchical Composites"*
Master in Composite Materials
Technical University of Madrid / AIRBUS
Professor: Dr. J. J. Vilatela

12. *"Procesos industriales"*
Máster en Ingeniería Industrial
Navarra University (TECNUN)
Professor: Dr. M. T. Pérez-Prado

13. *"Thermal and Thermo-mechanical characterization"*
Master in Materials Science and Engineering
Carlos III University of Madrid
Professor: Dr. S. Milenkovic

5.4. Institutional activities

14. *Member of the Severo Ochoa Centres and María de Maeztu Units Alliance (SOMM Excellence Alliance)*

15. *Member of the European Materials Modelling Council (EMMC)*

16. *Member of the European Materials Characterization Council (EMCC)*

17. *Member of the European Energy Research Alliance (EERA)*

18. *Member of the European Technology Platform for Advanced Engineering Materials and Technologies (EUMAT)*

19. *Member of the Batteries European Partnership Association (BEPA)*

20. *Member of the European Technology and Innovation Platform Batteries Europe*

21. *Local Contact Point of the EURAXESS pan-European initiative*

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

23. *Member of the Spanish Aerospace Platform (PAE)*

24. *Member of the Spanish Technological Platform for Advanced Manufacturing (MANUKET)*

25. *Member of the Madrid Aerospace Cluster (MAC)*

26. *Member of the Network of Research Laboratories of Comunidad de Madrid (REDLAB)*

27. *Member of the Spanish Railway Technological Platform (PTFE)*

28. *Member of the Spanish Energy Storage Technological Platform (BatteryPlat)*

29. *Member of the Spanish Technological Photonics Platform (Fotónica21)*

30. *Member of the Spanish Association of Foundations (AFE)*

31. *Member of the Spanish Association of Composite Materials (AEMAC)*

32. *Member of the European Aeronautics Science Network (EASN)*

5.5. Individual participation in committees and other institutions

1. *Member of the European Materials Modelling Council (EMMC).* Prof. J. Segurado

2. *Member of the European Materials Modelling Council (EMMC).* Dr. D. Tourret

3. *Member of the European Materials Characterization Council (EMCC). Dr. J. Molina*

4. *Member of Batteries Europe WG2.* Dr. J. J. Vilatela

5. *Program coordinator, Structural Materials, Spanish National Science Foundation (AEI).* Dr. M. T. Pérez-Prado

6. *Vice president of SEMNI (Spanish Association for Numerical Methods in Engineering).* Prof. I. Romero

7. *Member of the Scientific Board, European Space Agency (ESA).* Dr. M. T. Pérez-Prado

8. *Member of the Strategic Advisory Board, Fundación Gadea Ciencia,* Dr. M. T. Pérez-Prado

9. *Member of the Scientific Board and of the Strategic Advisory Board, NOMATEN Center of Excellence.* Dr. M. T. Pérez-Prado

10. *Member of the Scientific Board, IRT Jules Verne.* Dr. M. T. Pérez-Prado

11. *Member of the International Technology Advisory Board, IRT Saint Exupéry, France.* Prof. J. Llorca

12. *Member of the Early Career Researcher Board of IOP Multifunctional Materials.* Dr. J. J. Vilatela

13. *Chair, European Mechanics of Materials Conference Committee.* Prof. J. Llorca

14. *Executive editor, Modelling and Simulation in Materials Science and Engineering.* Prof. J. Llorca

15. *Fellow of Royal Society of Chemistry, UK.* Dr. D-Y. Wang

5.6. Outreach

1. *Organisation of the "1st open PhD day" at IMDEA Materials.* January 2020.

2. *Speaker at the "Women in 3D printing" Madrid chapter visit at IMDEA Materials.* March 2020. Dr. C. Pascual, A. Fernández, A. Doñoro, L. Arévalo.

3. *Participation in the "European Researchers' night Madrid 2020 - Great Scientists on the big screen", promoted by Fundación Madri+d. November 2020.* Dr. M. Echeverry, Eugenia Nieto.

4. *Participation in the "Science Week Madrid 2020", promoted by Fundación Madri+d. November 2020.* J. de la Vega, C. Madrona, C. Galera, A. Álvarez, A. Fernández, Dr. D. Garoz.

5. *Organisation of primary-secondary school and bachelor-master students visits to IMDEA Materials Institute,* 3 visits during 2020 (over 100 students)

5.7. IMDEA Materials in the media

1. *Andamios de magnesio en 3D para tratar grandes fracturas óseas.* Prof. J. Llorca. RNE
2. *Nuevos materials para baterías.* Dr. J. J. Vilatela. RNE
3. *El silicio es la tecnología clave para las nuevas baterías.* Dr. J. J. Vilatela. RNE
4. *La CE apuesta por tecnología española en el desarrollo del silicio en láminas para baterías.* Dr. J. J. Vilatela. RNE
5. *Impresión 3D de materiales.* Dr. M. T. Pérez-Prado. RNE
6. *Hoy por hoy, interview to Dr. J. J. Vilatela.* Cadena SER
7. *Crean una estructura biodegradable impresa en 3D para regenerar huesos rotos.* Prof. J. Llorca. National Geographic España
8. *Diez investigaciones "made in Madrid" de las que está pendiente todo el planeta ciencia.* Drs M. T. Pérez-Prado, J. M. Molina-Aldareguia, R. Costa and J. J. Vilatela; Profs. J. M. Torralba and I. Romero. TeleMadrid
9. *Metals testing for aerospace under the microscope.* Prof. J. Segurado. Aerospace Testing International
10. *IMDEA Materials and Hexagon Partner for Next Gen Metal Simulation Tech.* Prof. J. Segurado. 3DPRINT.COM
11. *SORCERER: Clean Sky wizardry for multifunctional aircraft composites.* Dr. J. J. Vilatela. Composites World
12. *ITP Aero e IMDEA Materiales desarrollan un programa de I+D para simular la fabricación en 3D pionero en el mundo.* Dr. D. Tourret. Actualidad Aeroespacial
13. *Desarrollan un silicio flexible que revolucionará los vehículos eléctricos.* Dr. J. J Vilatela, Notiweb Madri+d
14. *New aviation fabrics serve dual structural and electrical roles.* Dr. A. Mikhalchan. CORDIS
15. *Sobre la Endogamia.* Prof. J. M. Torralba. Universidad, sí
16. *El sistema de ciencia e innovación, principales problemas y algunas soluciones.* Prof. J. M. Torralba. Universidad, sí
17. *¿Merece la pena hacer el doctorado en España?* Prof. J. M. Torralba. Universidad, sí
18. *Si el futbol se rigiera por las leyes de la ciencia o la universidad.* Prof. J. M. Torralba. Universidad, sí

Comunidad de Madrid

EUROPEAN UNION
STRUCTURAL FUNDS

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