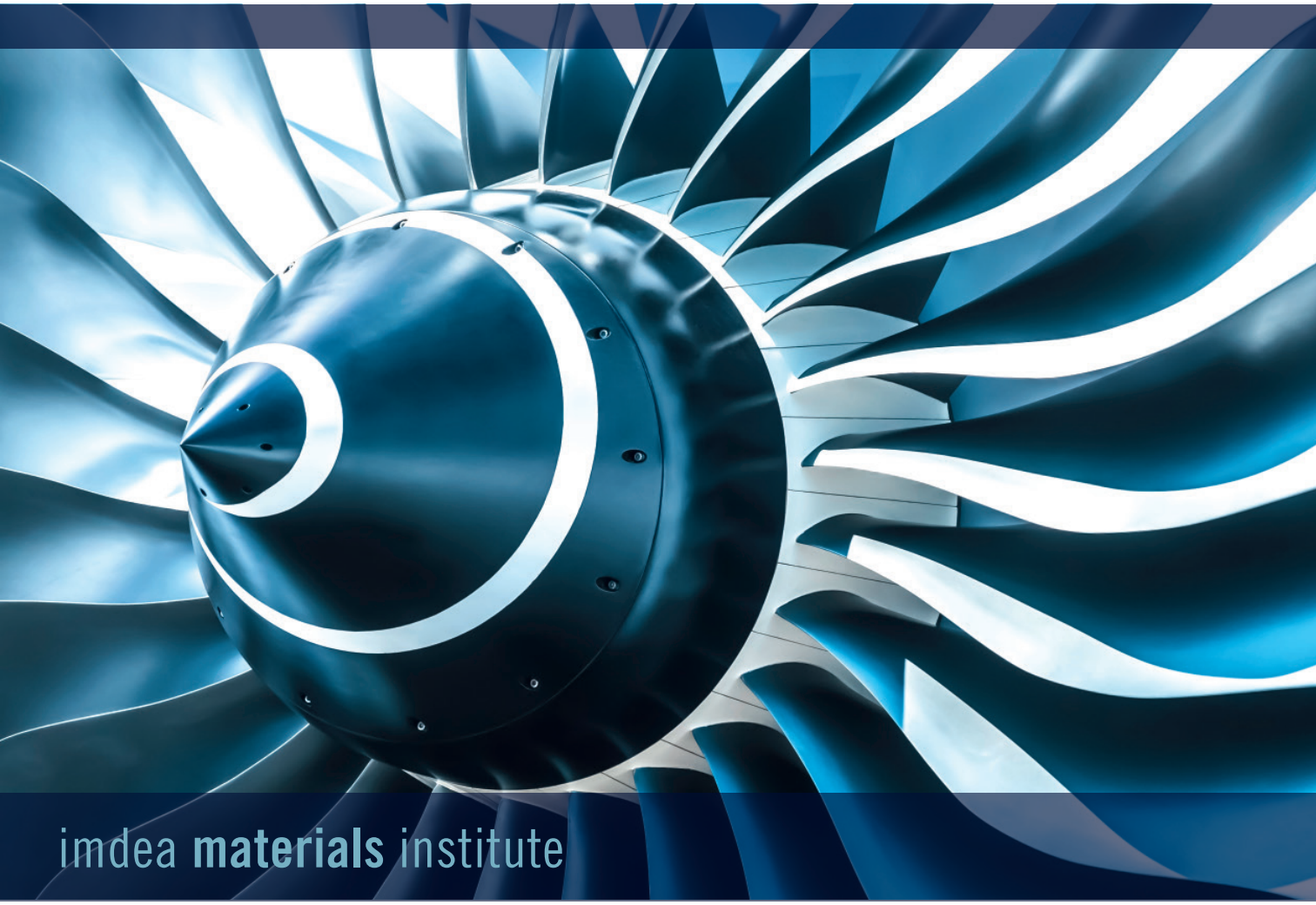
institute imdea materials



imdea **materials** institute

annual report

2019

www.materials.imdea.org

Ignacio Romero
Director, IMDEA Materials Institute
March 2020

annual report
2019
www.materials.imdea.org

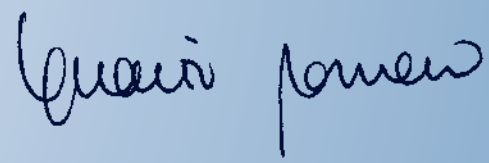
When perusing through this annual report one gets the clear impression that these are the results of a mature research institution, one with established groups and a well-identified direction. Shortly after its twelfth anniversary, this status has been officially recognised by the Spanish Government, and the Institute has been awarded the *María de Maeztu* seal of excellence for medium-sized research units.

This is no small step. IMDEA Materials joins now the exclusive SOMMa (*Severo Ochoa* and *María de Maeztu*) alliance, consisting of the top research centres and units in Spain. It is a recognition of the excellent research done in our Institute during the past decade. Also, it provides funding to develop an ambitious research project, one that will increase our excellence and visibility in Materials Science and Engineering. It will strengthen our current capacities and help us to open new research lines.

This report proves the excellent research performed in the Institute during the last year. The number of people working in the centre has levelled off —yet another sign of its maturity— while the impact, as measured by citations, has grown over 40% in one year. Remarkably, whereas the amount of executed funding is almost the same as in our best year ever, the funding attracted during 2019 has exceeded any previous year, ensuring the scientific activities for the near future.

The report also sets out the increasing number of international scientific collaborations with companies, research groups, and universities. The international visibility of our researchers —and the Institute— keeps growing and international projects are now our main source of competitive funding.

During 2019 we have also been working in two important documents. First, an ethics code that puts in writing our commitment to excellence in all our activities and behaviour; second, a *Roadmap* that will help up navigate the upcoming four years, clarifying our strategic goals and making us aware of potential difficulties that we will face along the way. The *María de Maeztu* research program is a piece of the puzzle that fits with other economic and personnel considerations. One conclusion is clear: the coming years will be extremely exciting for our centre and we will face some of the challenges that come with age, plus unexpected ones. We have an outstanding team of researches and staff, and we look forward to this new stage with confidence.



words from the director...

annual report 2019

www.materials.imdea.org

editor
IMDEA Materials Institute

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base 12 diseño y comunicación

D.L.
M-12730-2020

contents

about us

The IMDEA Materials Institute, one of the seven Madrid Institutes for Advanced Studies (IMDEA), is a public research centre founded in 2007 by Madrid's regional government. The goal of the Institute is to do research at the forefront of 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

The 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 with particular emphasis in transport and energy.

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

Societal Challenges

people

The core strength of the Institute is its international **research team, consisting of talented researchers from 20 different nationalities,** which carries out new scientific discoveries in Materials Science, and foster the development of emerging technologies.

103 researchers

20 nationalities

42% PhDs

53% foreign researchers

16 research groups

laboratory

The facilities of IMDEA Materials Institute

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

2.640 m^2 of research labs

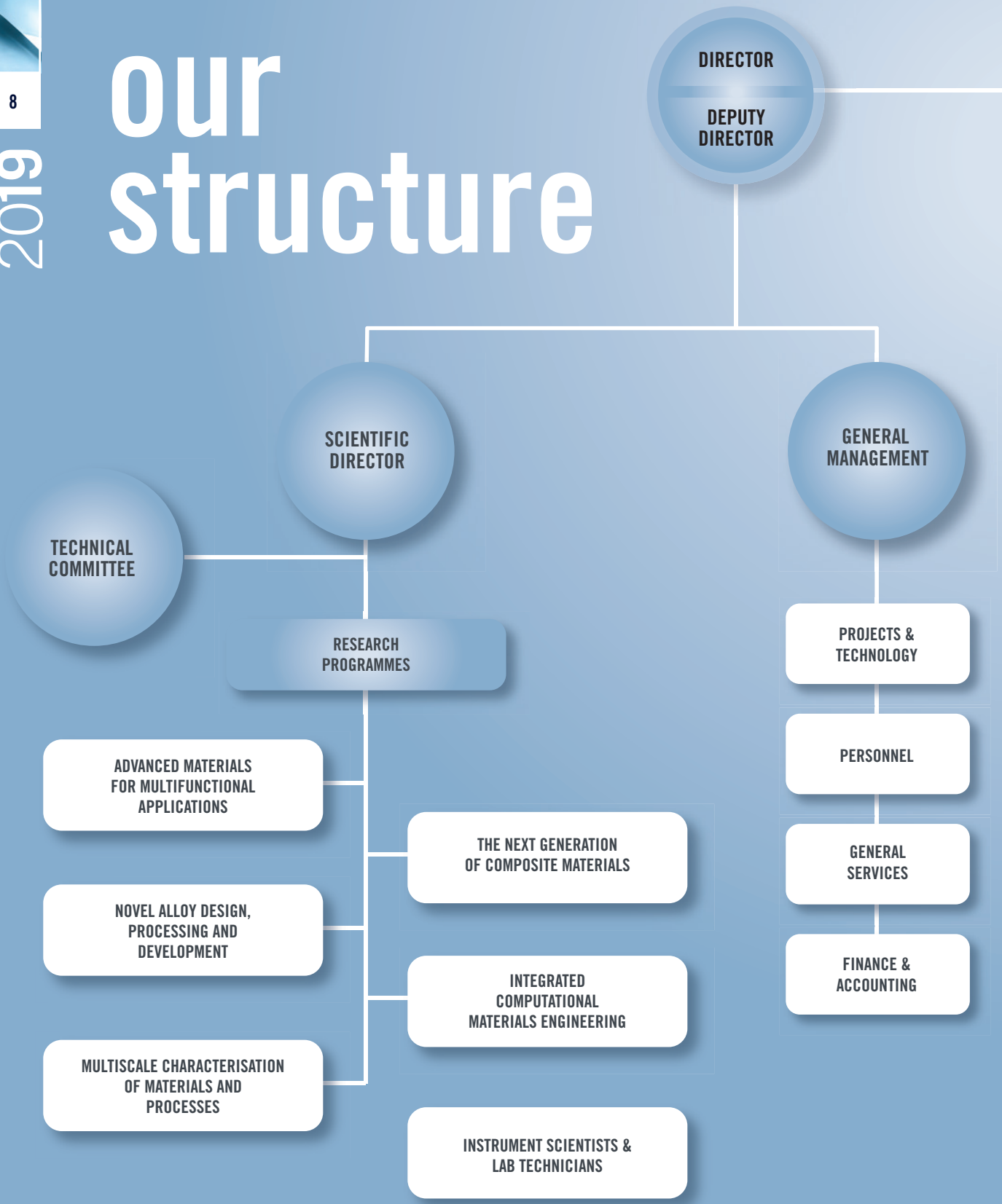
4 pilot plants

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

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

technology

our structure



BOARD OF TRUSTEES

CHAIRMAN OF THE FOUNDATION

To be appointed

VICE-CHAIRMAN OF THE FOUNDATION

Excmo. Sr. D. Eduardo Sicilia Cavanillas
Counsellor of Science, Universities and Innovation
Madrid Regional Government

PERMANENT TRUSTEES (REGIONAL GOVERNMENT)

Excmo. Sr. D. Eduardo Sicilia Cavanillas
Counsellor of Science, Universities and Innovation
Madrid Regional Government

Ilma. Sra. Dña. María Luisa Castaño
General Director of Research and Technological Innovation
Madrid Regional Government

Sra. Dña. Barbara Fernandez-Revuelta
Deputy General Director of Research and Technological Innovation
Regional Ministry of Science, Universities and Innovation
Madrid Regional Government

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Fundación para el conocimiento (Madri+d)

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Madrid Regional Government

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Mr. Luis Miguel Méndez Llatas
Advanced Materials Advisor
Repsol Technology Center

Prof. Manuel Doblaré Castellano
Professor
University of Zaragoza

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Professor Technical University of Madrid (UPM). Spain

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Vice Chancellor of Science Policy
Carlos III University of Madrid. Spain

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Professor
Cambridge University. UK

Prof. Dr. Andreas Mortensen
Vice-provost for Research
Professor
Ecole Federale Polytechnique of Lausanne (EPFL). Switzerland

Prof. Dr. Tresa Pollock
Professor
University of California at Santa Barbara. USA

Prof. Dr. Mauricio Terrones
Professor
Penn State University of Pennsylvania. USA

INDEPENDENT TRUSTEE

Mr. Pedro Escudero
Independent Consultant

COMPANIES TRUSTEES

AIRBUS, S.A.S.
Dr. José Sánchez Gómez. Head of Composite Materials Getafe. Madrid. Spain

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

INDUSTRIA DE TURBOPROPULSORES, S.A.
To be appointed

TOLSA, S.A.
Mr. Enrique Gómez Navarro. General Manager Madrid. Spain

SECRETARY

Mr. Alejandro Blázquez

SCIENTIFIC COUNCIL

Prof. Dr. Brian Cantor
Vice-chancellor
University of Bradford. UK

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Head of the Composites and Coating Group
Professor
Cambridge University. UK

Prof. Dr. Andrew I. Cooper
Director, Materials Innovation Factory
University of Liverpool. UK

Prof. Dr. William A. Curtin
Director Institute of Mechanical Engineering
Ecole Federale Polytechnique of Lausanne (EPFL). Switzerland

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Director Centre for Advanced Materials Technology (CAMT)
Professor
University of Sydney. Australia

Prof. Manuel Doblaré
Professor
University of Zaragoza. Spain

Prof. Dr. Tresa Pollock
Professor
University of California at Santa Barbara. USA

Prof. Dr. Andreas Mortensen
Vice-provost for Research
Professor
Ecole Federale Polytechnique of Lausanne (EPFL). Switzerland

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Independent Consultant

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Director International Center for Numerical Methods in Engineering (CIMNE)
Professor
Universidad Politécnica de Cataluña. Spain

Prof. Dr. Mauricio Terrones
Professor
The Pennsylvania State University. USA

Prof. Judith L MacManus-Driscoll
Professor
Cambridge University. UK

Prof. Michael Ortiz
Professor
California Institute of Technology. USA

in figures

human resources

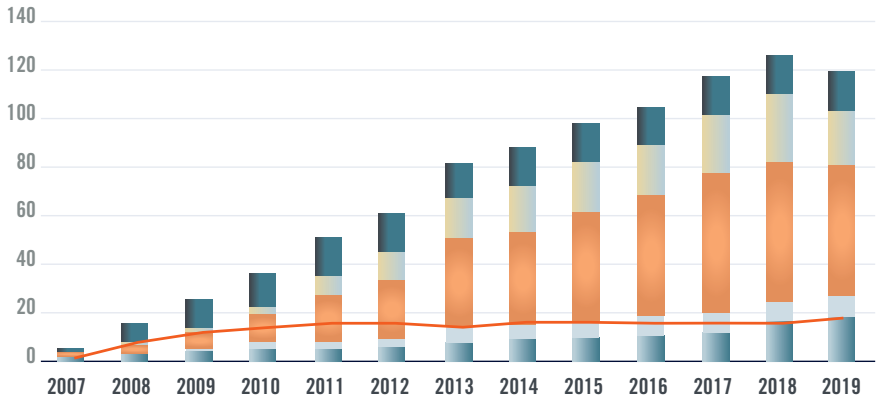
talent

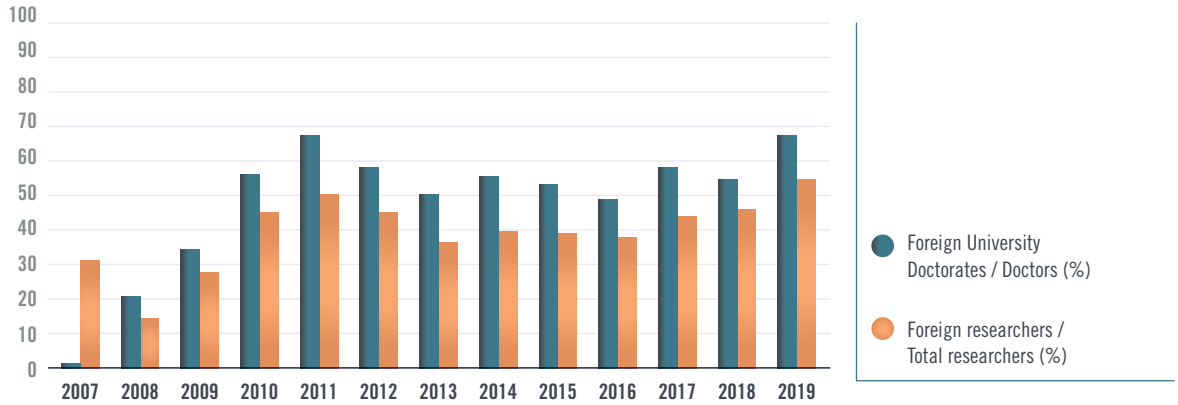
Talent attraction has been the key to the Institute´s **success**.

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**

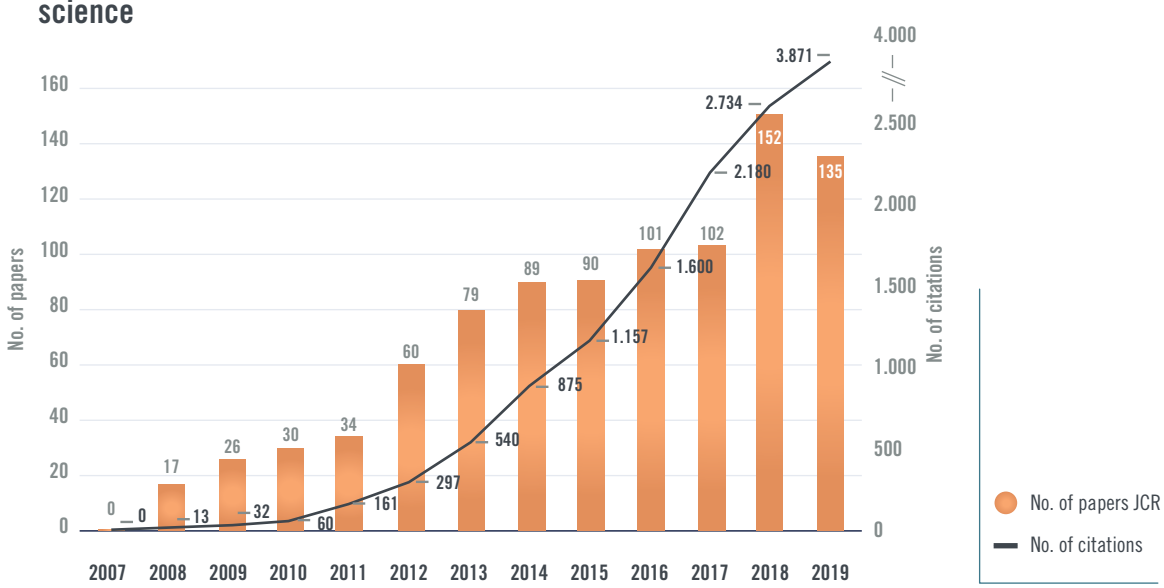
43 defended PhD theses since 2007

60 ongoing PhD theses

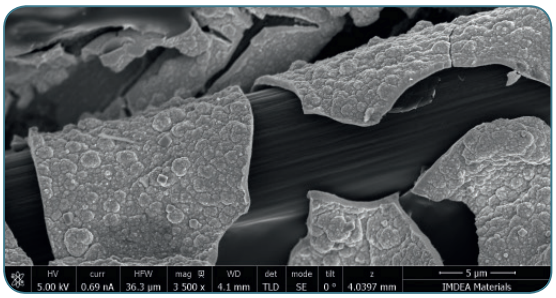
scientific results

science

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



2019



53 keynote/ invited talks

135 JCR papers

3871 number of citations

39 invited seminars and lectures

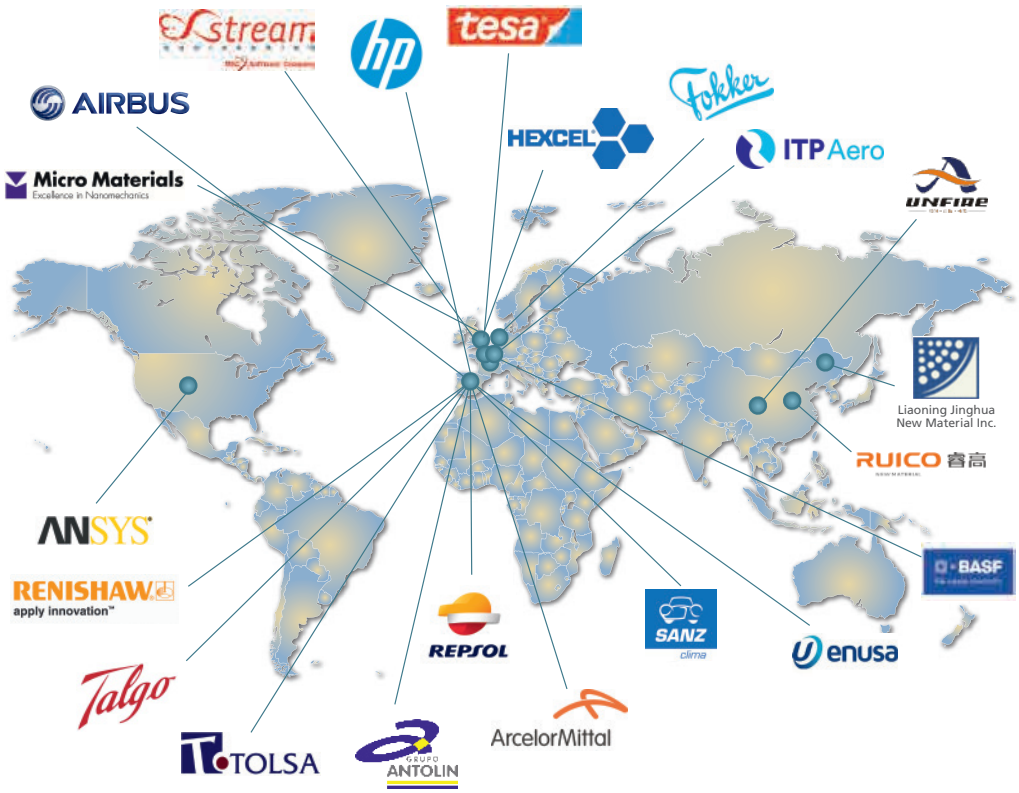
3 patent applications

10 patents in portfolio

transfer

The **unique scientific expertise and infrastructure** of IMDEA Materials Institute enables its research groups to collaborate with national and international industry **for the benefit of the Madrid´s region and its development as technological hub** in Europe.

Companies which had active collaboration with IMDEA Materials during 2019



IMDEA Materials Institute is establishing strategic partnerships with other research centres and universities around the world, which are internationally recognised in the field of Materials Science and Engineering. The goal is to create long-term collaboration frameworks of mutual benefit to develop exchange programmes of researchers and students, joint research projects and joint international PhD programmes.

International joint PhD supervision agreements

IMDEA Materials has established two agreements with foreign universities for joint supervision of doctoral students, who spend approximately two years in Madrid and another two abroad during their PhD studies.

UNIVERSITY OF TEXAS ARLINGTON

TEXAS A&M UNIVERSITY

Scientific/technological international partnerships

WASEDA University

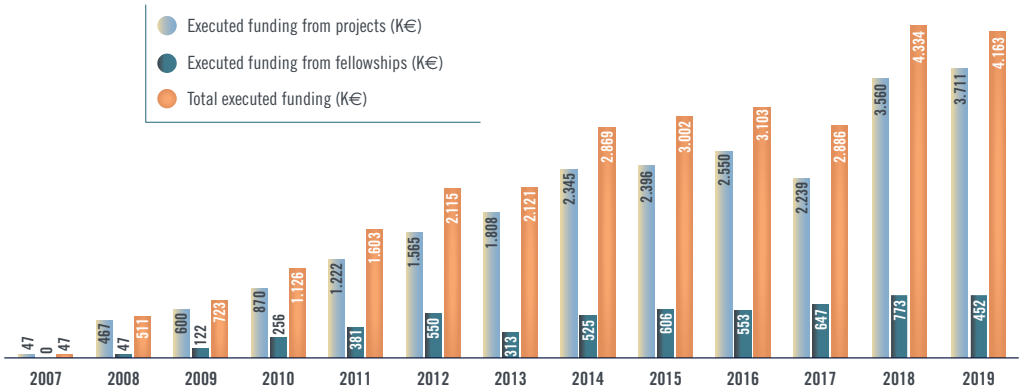
Waseda University, Japan - Energy-Next Initiative
Area of nanomaterials applied to energy

Spain-China joint research centre of advanced materials (JRCAM)
Area of advanced polymeric materials

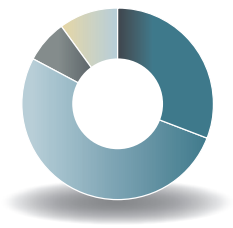
Members: IMDEA Materials Institute (Co-Director), Beijing University of Chemical Technology, Going Global Confederation of China Petroleum & Chemical Industry, Beihang University, Universidad Politécnica de Madrid, regional government of Aragón and the companies SANZ CLIMA and REPSOL.

projects and fellowships

Research activities are performed in the framework of R&D projects and fellowships, which are funded either by regional/national/ international agencies or through direct contracts with companies.



2019



- **International projects** 51%
- **National projects** 12%
- **Regional projects** 13%
- **Contracts with industry** 24%

63
R&D projects

3
ERC projects

14
R&D contracts with companies

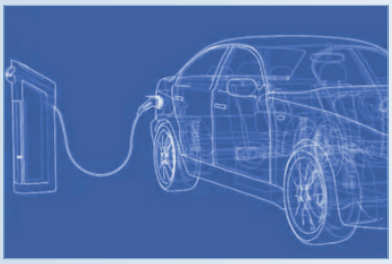
research

talent science transfer

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

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

Advanced Materials for Multifunctional Applications

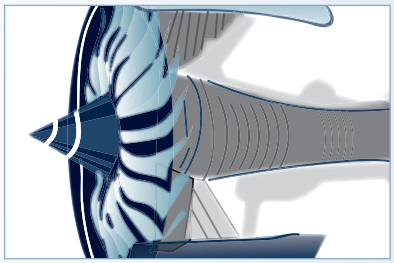


- Synthesis and integration of nanomaterials and polymer-based multifunctional nanocomposites
- New materials and strategies for electrochemical energy storage and conversion
- Hybrid optoelectronic materials and sustainable lighting devices
- Computational and data-driven materials discovery

The Next Generation of Composite Materials

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

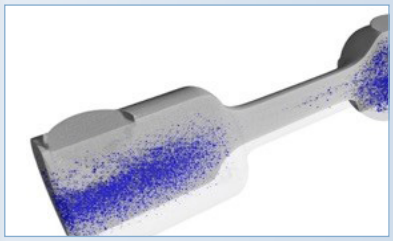
Novel Alloy Design, Processing and Development



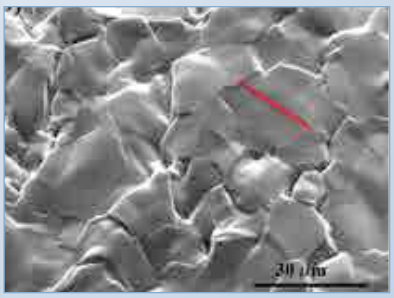
- Structural alloys: light alloys, high temperature alloys and high strength steels
- Characterisation of microstructure and mechanical behaviour
- Advanced manufacturing: solidification and casting, physical simulation of metallurgical processes (rolling, forging, extrusion...)
- Powder metallurgy and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

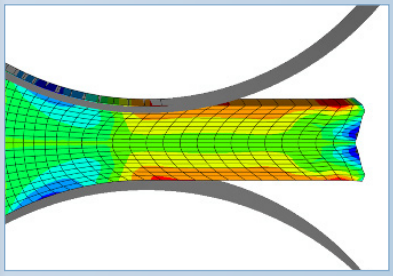


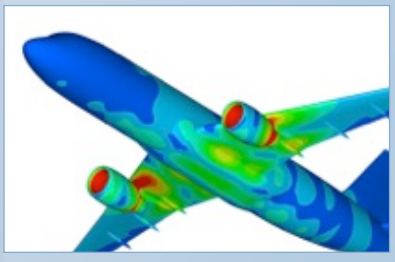
- **4D characterisation:** In-situ characterisation of deformation and processes across multiple length scales (750ºC)



Integrated Computational Materials Engineering

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



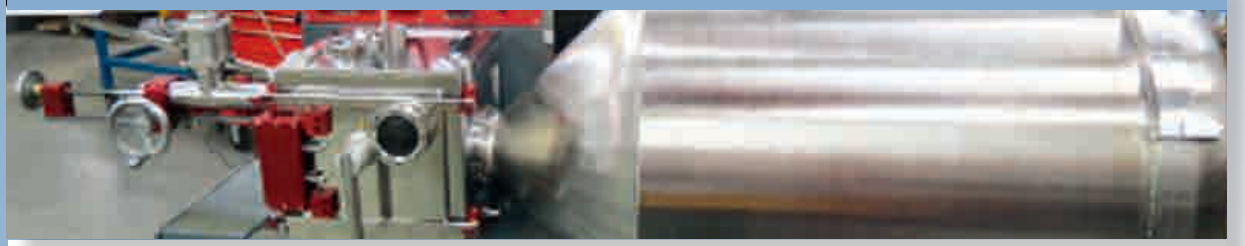


facilities

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.

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.

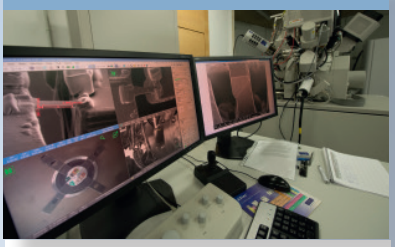
Energy storage and conversion devices

- 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.

Lighting devices

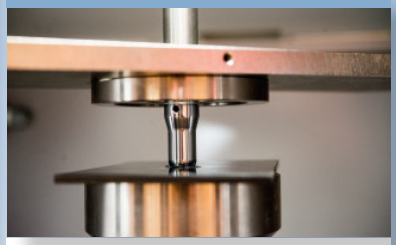
- Fabrication and characterisation of hybrid light-emitting diodes and thin-film lighting devices.
- Rack system consisting of 7 positions that are independently driven, while the luminance and chromaticity features are monitored over time via UV-VIS spectrophotometers coupled to integrated spheres.
- Station to measure spatial light distribution and temperature generation in a micrometre resolution over time.
- Rack system for measuring thin film lighting devices using different poling modes, while controlling luminance and chromaticity features over time using eye-corrected detectors
- Electrochemical impedance spectroscopy (EIS).

Microstructural and chemical characterisation



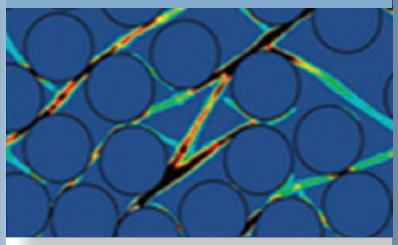
- 3D microscopy at different length-scales, including X-ray tomography, 3D-SEM, 3D-EDS and 3D-EBSD in the FIB and 3D-TEM and 3D-EDS in the TEM.
- In-situ mechanical testing of mininaturised samples in the X-ray tomography system as well as in the SEM and TEM.
- In-situ processing studies in the X-ray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

Mechanical properties



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

Simulation



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

Functional properties

Fire resistance

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

Thermal

- DSC, TGA and Hot Disk Thermal Conductivity 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.

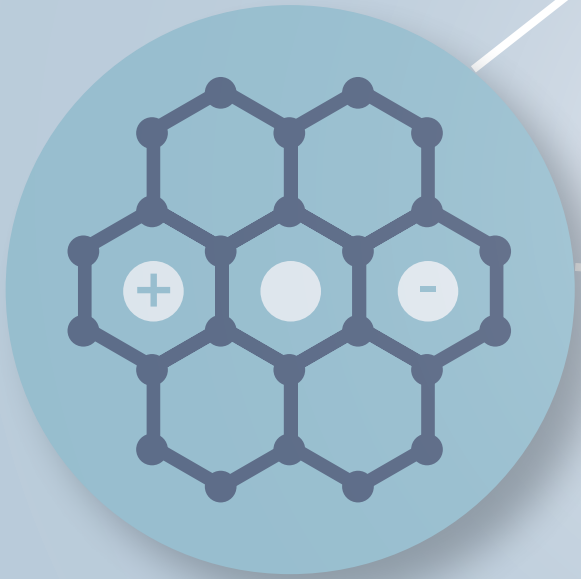
Photophysical

- UV-VIS absorption and emission spectrophotometers for solutions, thin films, and powders.
- Integrating spheres to measure diffuse reflectance and photoluminescence quantum yields.
- Electrochemical stations to perform static and time-resolved spectroelectrochemistry.
- Time-Correlated Single Photon Counting using a laser excitation module.

programme
Advanced Materials for Multifunctional Applications

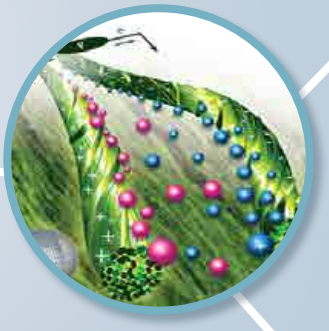
Goal and vision

The Programme on Advanced Materials for Multifunctional Applications at IMDEA Materials Institute combines expertise in design and synthesis of nano and molecular building blocks with their integration into macroscopic materials and devices. The guiding objective is to simultaneously realise various functions, including fire safety, high-performance mechanical properties and efficient energy management, amongst other properties. 45 researchers in the programme combine expertise spanning from *in silico* molecular design to fabrication of large energy storing devices.

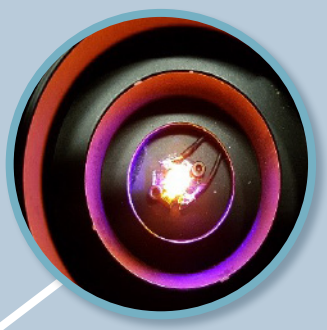


High Performance Polymer Nanocomposites

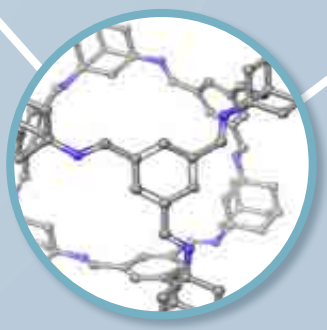
Electrochemical Energy Storage, Nanomaterials



Multifunctional Nanocomposites



Hybrid Optoelectronic Materials and Devices



Computational and Data-Driven Materials Discovery

Main research lines

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

- Synthesis 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.

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.

Bio-hybrid optoelectronics

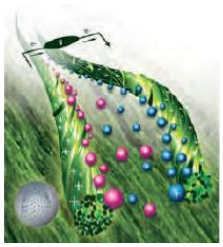
- Design of elastomeric color down-converting materials based on fluorescent proteins.
- Fabrication and analysis of single-point lighting and display systems.
- Further development towards bio-diagnosis and bio-reactor applications.

Electrochemical energy storage

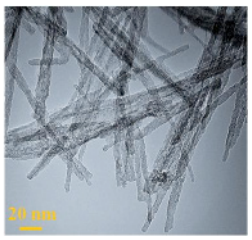
- Tailored designing of nanostructured electrode materials for electrochemical energy storage.
- Engineering of electrode-electrolyte interfaces for high-performance batteries and capacitors
- Spectroscopic and microscopic (in-situ and ex-situ) investigation of ion storage mechanism in energy storage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

Computational and data-driven materials discovery

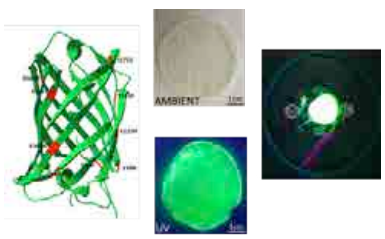
- Discovery of porous materials for energy applications (CO_2 capture, methane storage).
- Design of ionic liquids.
- Characterisation of nanoparticles and others.



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



Defect engineered electrodes.



Design of fluorescent protein for color down-converting filter for Bio-LEDs.

Fire-safety multifunctional materials.

Projects in focus

TOBEST / Functionalisation of natural brucite and its application in polymers

Funding: Liaoning Jinghua New Material Inc. P.R. China
Partners: IMDEA Materials Institute
Project period: 2019 - 2020
Principal Investigator: Dr. De-Yi Wang

This is the third phase of the continuous cooperation with the Liaoning Jinghua New Material Inc. The main objective of this project is to develop modified natural brucite powder for high performance polymer modification. It is expected that the modified brucite surface will have a certain coating layer to improve the interface interaction between the brucite particles and the polymer matrix, so as to promote the dispersion of brucite particles in the polymer matrix, and finally achieve the effect of improving Melt Flow Index (MFI), elongation at break and fire safety.

It will be achieved via selecting the appropriate commercial surface modifier, or synthesizing different kinds of new surface modifiers to modify the surface in situ under the appropriate temperature and high-speed stirring. The samples of modified polymers will be prepared by screw extrusion and injection molding. The effects of different polymers, different surface modifiers and different modification amount on the properties of polymers will be studied to determine the optimal conditions and to obtain the most competitive and high-quality flame retardants.

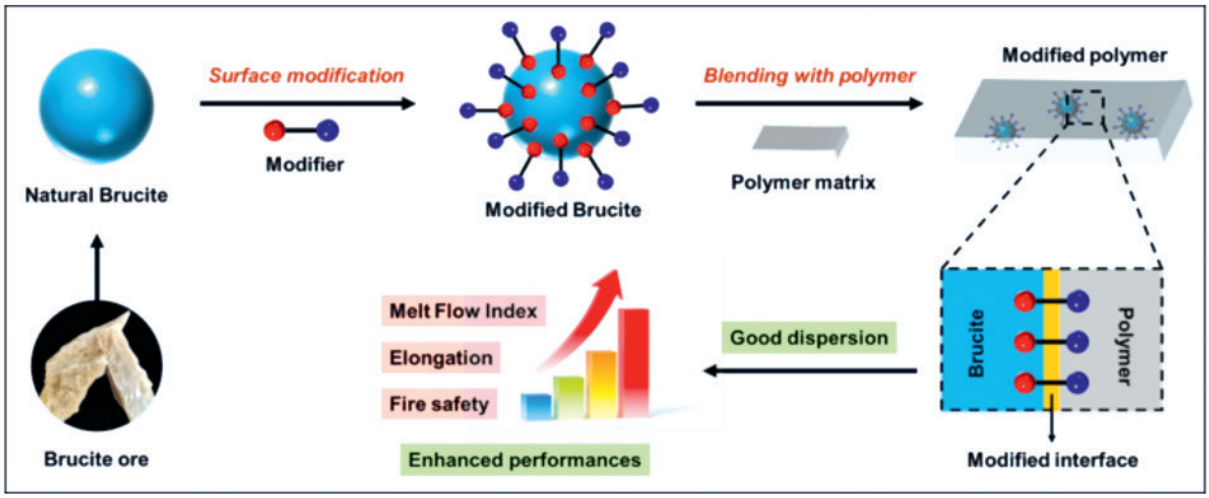


Figure 1. The whole process diagram of brucite powder modification and its application in polymer modification. Typically, the powder is generated from natural Brucite ore. Pristine natural powder is modified by some functional molecules (e.g. some special surfactants or saline) via high mixing equipment. The surface modification facilitates the good dispersion of brucite powder in the polymer matrix, enhancing the polymer performance, mainly MFI, LOI, and Elongation at break.

FotoArt-CM / New generation of multifunctional materials for artificial photosynthesis

Comunidad de Madrid

EUROPEAN UNION
STRUCTURAL FUNDS

Funding: Regional Government of Madrid. Technologies 2018
Partners: : IMDEA Energy Institute (Coordinator), IMDEA Materials Institute, IMDEA Nanoscience Institute, Madrid Institute of Materials Science (ICMM-CSIC), Institute of Catalysis and Petrochemistry (ICP-CSIC), Autonomous University of Madrid (UAM)
Project period: 2019-2022
Principal Investigator at IMDEA Materials Institute: Dr. Juan José Vilatela

FOTOART aims at making sustainable fuels and commodity chemicals by artificial photosynthesis, using affordable and sustainable materials, with solar energy the main energy source. This includes the conversion of CO_2 into products, nitrogen fixation and renewable hydrogen, which will be game changers in the fight against climate change. This project gathers scientific and industrial communities that will develop complementary technologies to harvest solar energy for the pursued chemical aims. FOTOART targets two synergistic S&T approaches: (i) photootocatalytic conversion and (ii) photoelectrochemistry with renewable power. The cornerstone of strategies proposed in FOTOART is the integration of intersectorial approaches on:

(1) Development of innovative and multifunctional materials from model to real systems, specifically designed for this challenging application: MOFs, carbon materials and hybrid inorganic-organic semiconductors;

(2) Combination of advanced theoretical calculations with experimental operando characterization tools for understanding the relationship between structure and reactivity;

(3) New advances in catalysis engineering with the design and construction of photo-/photoelectrochemical devices and solar reactors enabling the evaluation of the catalytic performance in artificial photosynthesis.

(4) Ultimately, the novel solar-to-chemical technologies will be integrated into the full value chain, integrating the capture and the final use of products.

A self-consistent strategy in cooperative research and training will be the most outstanding impact of the network. Specific network-wide training activities will complement specialized local courses, seminars.

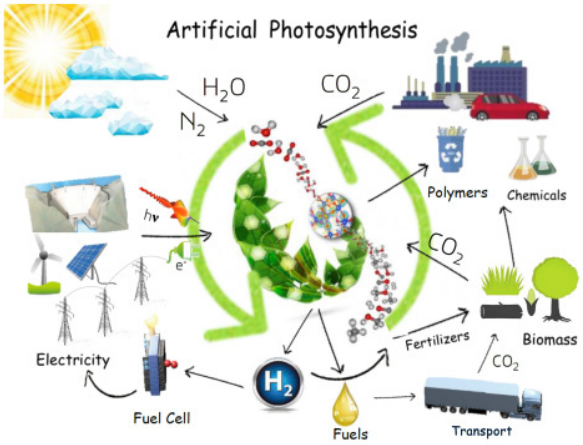


Figure 2. The FOTOART-CM concept.

IMDEA Materials is focused on two activities: i) the synthesis and characterization of functionalized CNT fibers to couple a myriad of electrocatalysts towards developing multifunctional electrodes (current collector/ catalysis) and ii) the use of spectro-electrochemical techniques to study charge transfer, transport and recombination processes in fully operative devices.

Scientific highlights

New nanostructured materials for high-rate Li-ion battery anodes: properties and lithium storage mechanism study by in-situ synchrotron X-ray scattering

There is an ever-increasing interest in new materials that can extend the current performance of battery electrodes materials in terms of longer cyclability, higher energy density and higher power density. Our research groups have established a route for the fabrication of high-performance anodes for rechargeable Li-ion batteries produced by nano structuring of transition metal oxides on a conductive support. In a recent work, we demonstrated a hybrid material of MnO_2 directly grown onto fabrics of carbon nanotube fibers, which exhibits notable specific capacities over 1100 and 500 mA h g^{-1} at discharge current densities of 25 mA g^{-1} and 5 A g^{-1}, respectively, with a Coulombic efficiency of 97.5%. Combined with 97% capacity retention after 1500 cycles at a current density of 5 A g^{-1}, both capacity and stability are significantly above literature data. Detailed investigations involving electrochemical and in situ synchrotron X-ray scattering studies reveal that during galvanostatic cycling, MnO_2 undergoes an irreversible phase transition to $LiMnO_2$, which stores lithium through an intercalation process, followed by a conversion mechanism and pseudocapacitive processes. This mechanism is further confirmed by Raman spectroscopy and X-ray photoelectron spectroscopy. The fraction of pseudocapacitive charge storage ranges from 27% to 83%, for current densities from 25 mA g^{-1} to 5 A g^{-1}. The firm attachment of the active material to the built-in current collector makes the electrodes flexible and mechanically robust, and ensures that the low charge transfer resistance and the high electrode surface area remain after irreversible phase transition of the active material and extensive cycling.

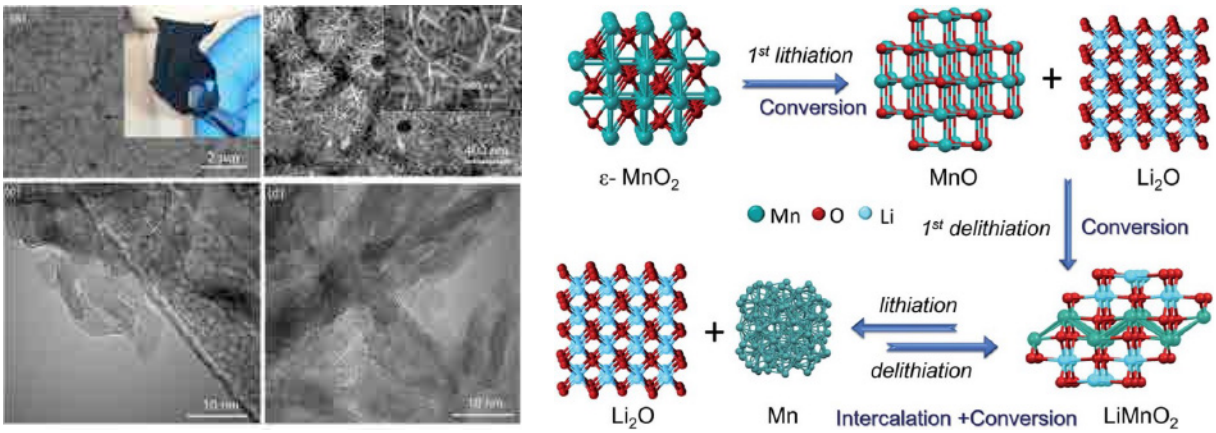


Figure 3. Hybrid materials of MnO_2 grown on CNT fibres as battery electrodes. (a)-(d) optical and electron micrographs of the nanostructured material. (e) Schematic diagram for the structural transformation of MnO_2 observed by in situ XRD measurements.

Reference: M. Rana, V.S. Avvaru, N. Boaretto, V. Oshea, R. Marcilla, V. Etacheri, J.J. Vilatela. *High rate hybrid MnO2@CNT fabric anodes for Li-ion batteries: Properties and a Lithium storage mechanism study by in situ synchrotron X-ray scattering.* **Journal of Materials Chemistry A 7**, 26596-26606, 2019.

Hierarchical Strategy for Simultaneous Improvement of Mechanical and Fire-Safety Properties of Polymer Composites with Phosphonate-Loaded MOF Additives

Flame retardant (FR) additives are commonly used to improve fire-safety of synthetic polymers, which are widely employed in manufactured consumer goods. The incorporation of a FR in a polymer typically leads to deterioration of its mechanical properties. It also manifests itself in a non-negligible volatile organic compounds (VOCs) release, which in turn increases environmental risks carried by both the application and disposal of the corresponding consumer goods. We presented a hierarchical strategy for the design of composite materials, which ensures simultaneous improvement of both mechanical and fire-safety properties of polymers while limiting the VOC release. Our strategy employs porous metal organic framework (MOF) particles to provide a multifunctional interface between the FR molecules and the polymer. Specifically, we demonstrated that the particles of environmentally friendly HKUST-1 MOF can be infused by a modern FR - dimethyl methylphosphonate (DMMP), and then embedded into widely used unsaturated polyester. The DMMP-HKUST-1 additive endows the resulting composite material with improved processability, flame retardancy and mechanical properties. Single-crystal X-ray diffraction, thermogravimetric analysis and computational modeling of the additive suggests the complete pore filling of HKUST-1 with DMMP molecules being bound to the open metal sites of the MOF.

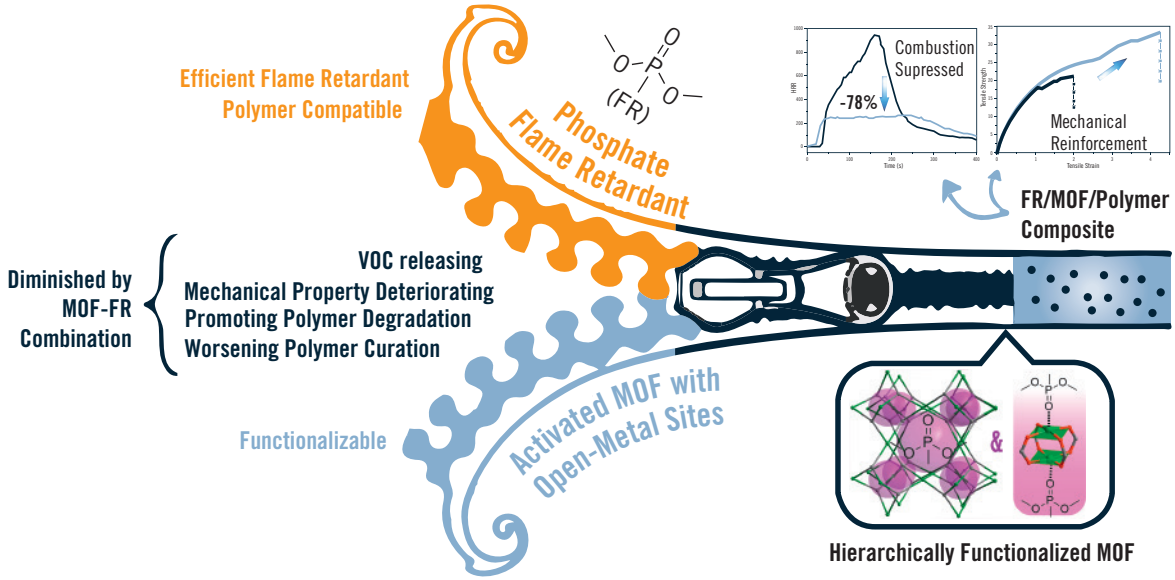
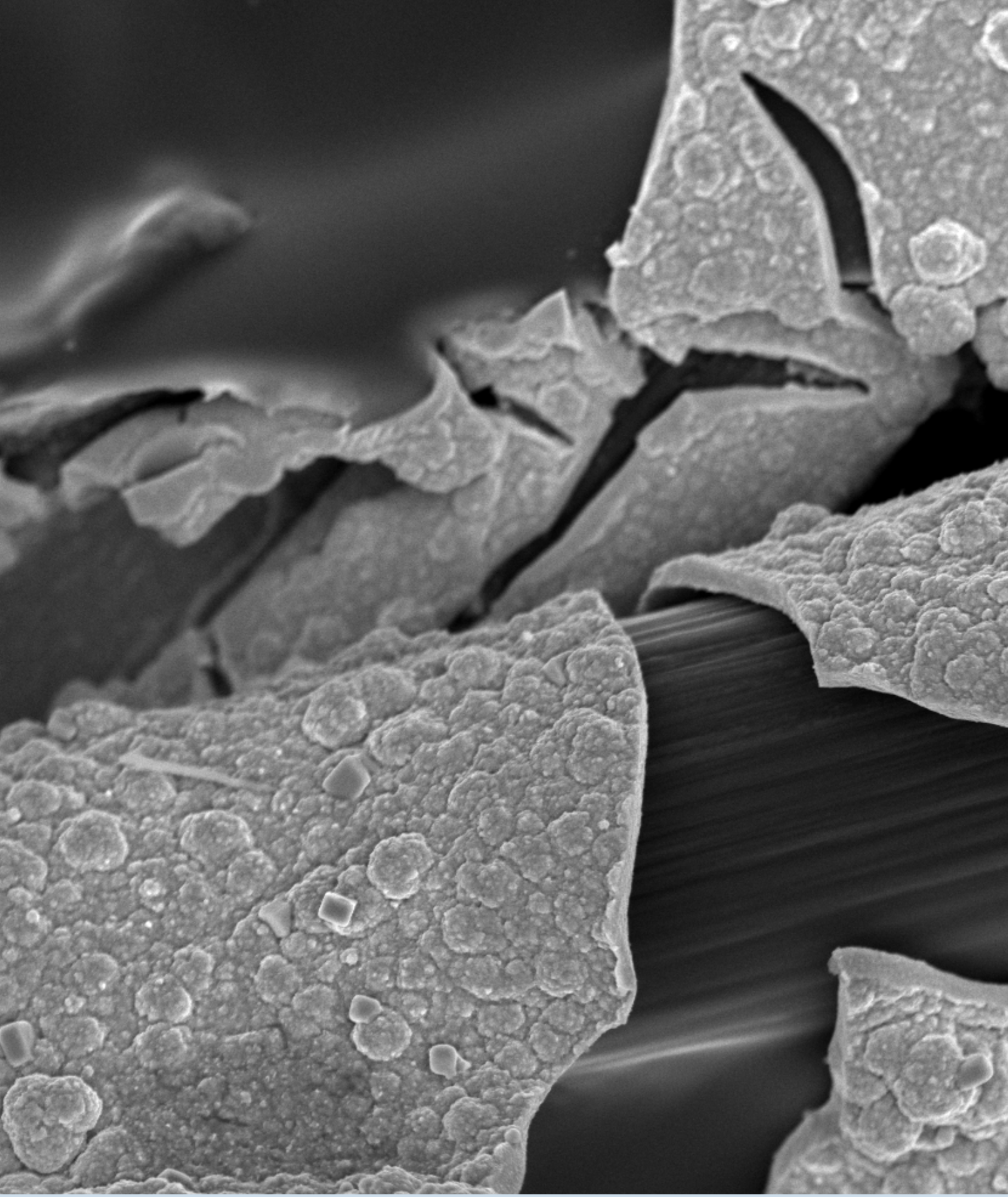


Figure 4. Schematic depiction of merging properties of a polymer and a flame retardant-filled MOF particles.

Reference: X.-L. Qi, Dong-Dong Zhou, J. Zhang, S. Hu, M. Haranczyk* and D.-Y. Wang*. **ACS Appl. Mater. Interfaces 11**, 22, 20325-20332, 2019.



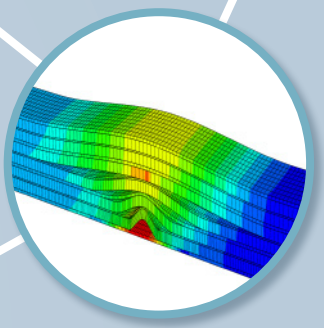
programme
The Next Generation of Composite Materials

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.

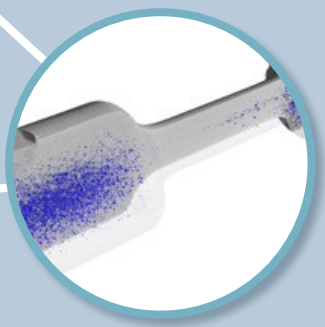
High Performance Polymer Nanocomposites

Multifunctional Nanocomposites



Design & Simulation of Composite Structures

Structural Composites



X-Ray Characterisation of Materials

Nanomechanics

Main research lines

Processing of high performance composites

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

Recycling 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

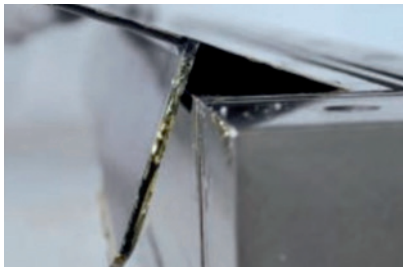
- Multiscale strategies for design and optimisation of composite materials and structures. Behaviour of composite materials and structures under high velocity impact (ice, metallic fragment or blade). Crash-worthiness and failure of composite structures. Effects of defects.

Virtual processing of composites

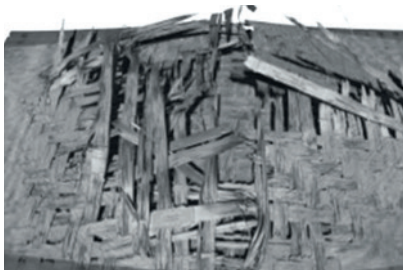
- Manufacturing process simulation. Multiphysics models for manufacturing including forming, injection/infusion process as well as curing. Characterisation of processing parameters.

Digital technologies for structural composites

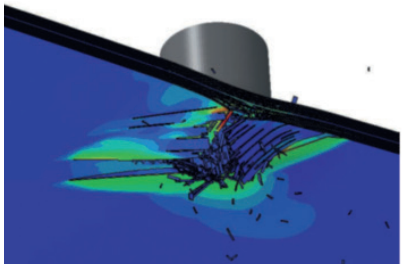
- Methods of artificial intelligence for optimization of composite manufacturing and structural performance. Sensors and process controls. Digital twins and hybrids.



Manufacturing of structural composites.



Multifunctional composites (e.g. lightning impact).



Multiscale virtual testing and processing.

Projects in focus

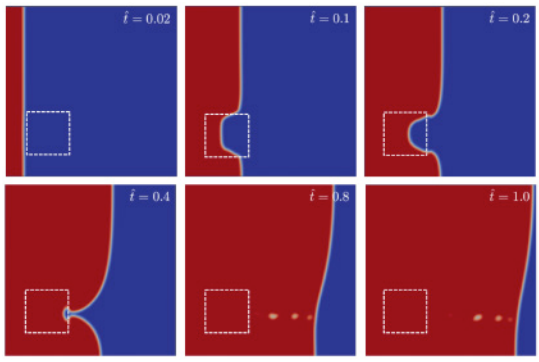
TEMACOM / Advanced manufacturing technologies for the new generation of composite materials

Comunidad de Madrid

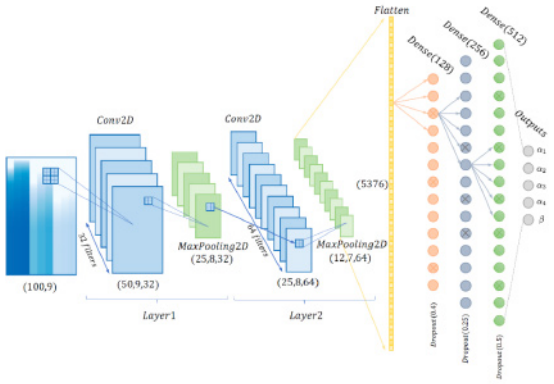
EUROPEAN UNION
STRUCTURAL FUNDS

Funding: Regional Government of Madrid, Open Innovation Hubs
Partners: Airbus Operations (Coordinator), Zinkcloud, Obuu Tech, Foundation for the Research Development and Application of composite materials (FIDAMC), IMDEA Materials Institute
Project period: 2019 – 2022
Principal Investigator: Prof. Carlos González

Nowadays, carbon fibre composite materials are in widespread use in structural applications in sectors such as transportation, sports, construction, civil engineering, or power generation. One of the main drawbacks limiting their use extension lies in the high manufacturing costs compared to other structural materials. Undoubtedly, the reduction in manufacturing costs involves a greater automation of manufacturing techniques, as well as the final optimization of the composite part based on innovative computer simulation strategies. One of the long-term objectives present in this industry is the possibility of designing and optimizing composite materials and their structures based on simulation techniques, before they proceed to manufacture so that the traditional concept of testing-and-error will be replaced with more effective concepts based on right-first-time. IMDEA Materials´ contribution in TEMACOM project will focus on two main objectives highly aligned with those previously mentioned. On one hand, the analysis by Virtual Processing of the manufacturing defects, as wrinkles, generated during thermoforming of fresh prepregs based on reliable finite element models accounting for the physical phenomena involved such as ply sliding and deformation. The purpose is to develop tools able to predict the occurrence of ply wrinkles in terms of location and amplitude as well as the determination of their effect in the final composite material performance. On the other hand, IMDEA Materials´ team will also address the prompt detection of defects occurring during injection/infusion of dry preforms by artificial intelligence techniques based on deep learning techniques similar to other technological disciplines as automatic driving of vehicles, voice and image recognition or automatic detection of tumors. Figure 1a) shows the flow (left to right) distortion caused by a region with different permeability. Mold sensors will be used for a fast detection of such processing disturbances using deep neural networks, see Figure 1b), so interaction on-the-fly during processing will be possible. TEMACOM has been funded through the Innovation Hubs Program of the Regional Government of Madrid.



(a)



(b)

Figure 1. a) Flow distortions caused by the presence of a dissimilar permeability region, b) Deep learning neural network used to detect flow disturbances during injection of dry preforms.

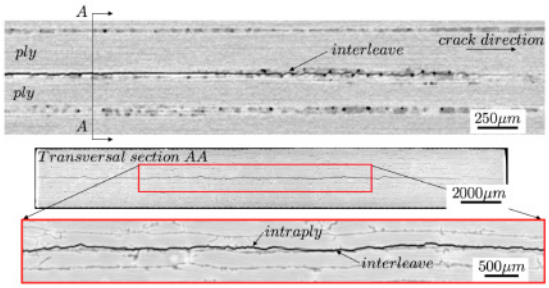
Scientific highlights

Dynamic behavior of composites: Coupling tests and simulations

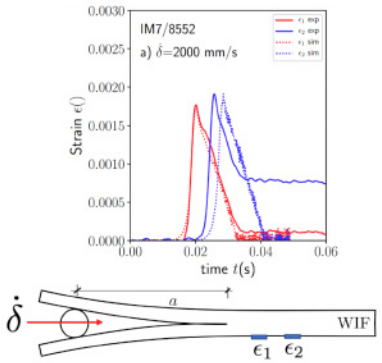
The use of polymer-based composite materials in aircraft structures has increased consistently in the last decades and today they represent up to 50% in weight for wings, fuselage sections and tail surfaces in the latest generation of commercial aircrafts. However, the use of such composites in other parts of the aircraft that could benefit from their low weight, such as the fan blades of engines and nacelles, is progressing, but at more subdued rate and this could be partially attributed to the lack of a general knowledge regarding the mechanical response of composite laminates under dynamic loading or impacts.

The dynamic behavior of structural composites is being investigated at IMDEA Materials within the DYNACOM Project. The main aim of the DYNACOM (Dynamic behavior of composite materials for next generation aero engines) training network is to set up a European Industrial Doctorate (EID) programme on the design of the next generation of structural composite materials for high strain rate applications (the next generation of aero engines mainly).

Within this project context, the dynamic behavior of prepregs laminates under interlaminar loading was studied by using the wedge-insert fracture method (WIF) with double cantilever beam specimens (DCB) at high speed (up to 2000 mm/s) with a Gleeble 3800-GTC thermal-mechanical physical system[1]. The standard prepreg materials systems (e.g. IM7/8552) did not exhibit strain rate dependence in the range analyzed. However, last prepreg generation containing interlaminar tougheners (e.g. IM7/M91) showed a significant increase of the toughness with the loading speed up to some extent. X-ray tomograms of the tested specimens revealed irregular crack propagation caused by the presence of toughening particles at the interleaves, Figure 2a). Finite element models using the cohesive approach were developed to check the consistency of the dynamic measurements and validate the data reduction methods used, Figure 2b). Such models, once calibrated with experimental results, can be used to ascertain the effect of strain rate on the mechanical performance of composite materials under dynamic loading conditions.



(a)



(b)

Figure 2: a) X-ray CT sections of the WIF specimen tested at high speed showing crack meandering due to the presence of secondary toughening particles, b) Model of the WIF specimen with comparison of the strain signals time evolution.

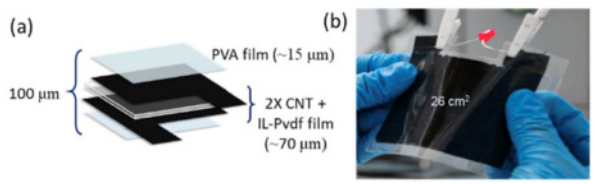
[1] M.A. Riezzo, M. Simmons, B. Russell, F. Sket, V. Martínez, C. González. *Dynamic characterisation of interlaminar fracture toughness in carbon fibre epoxy composite laminates.* **Composites Part A: Applied Science and Manufacturing 126**, 2019.

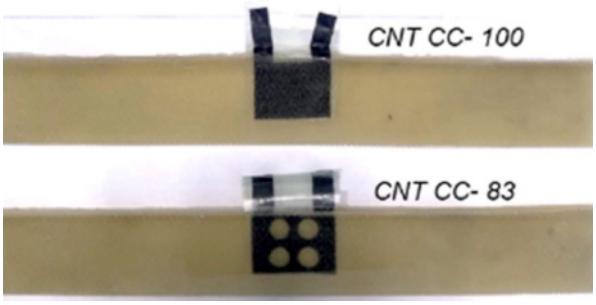
Integration of energy storage devices in structural laminates[2]

One of the current scientific and technological trends in structural composites is the incorporation of new functionalities as thermal/electrical conductivity or energy harvesting capacities to classical laminates. However, the inclusion of any internal conductive layer with capacitive storage will produce will produce undoubtedly detrimental effects as delaminations and lack of strength.

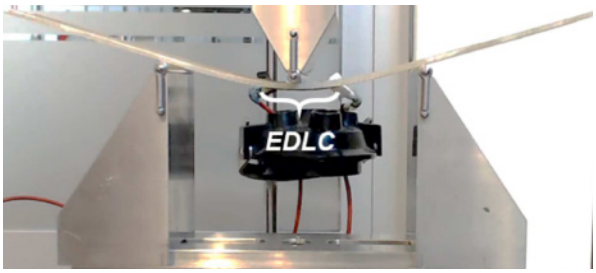
Structural laminates with integrated electric double layer capacitive storage were designed and produced at IMDEA Materials using resin infusion of dry fibre preforms, Figure 3a), b) and c). An internal carbon nanotube non-woven fabric working as electrodes/current collectors and a polymer ionic liquid membrane was used as energy storing layer. To avoid/mitigate the effect caused by the internal layer acting as a delamination, the energy storing layer was patterned with holes which after infusion act as resin plugs for mechanical interconnection between layers, a procedure similar to riveting. Finite element modelling was used to optimize rivet shape and areal density on the interlaminar shear properties of the laminate. It should be highlighted that the aforementioned method of inclusion of CNTF fabric and polymer electrolyte for energy storage is carried out without any metallic current collectors.

The robustness of the structural supercapacitor composite was evaluated by three-point bending (see Figure 3d) tests including progressive deflection, repeated load/ unload cycles up to fracture, combined with in/ex situ electrochemical measurements. The multifunctional material developed showed no appreciable degradation of its electrochemical properties, a consequence of the use of the CNTF fabric electrode as current collector. The use of CNT fibre current collector increases energy/power density and the overall figures of merit in energy-storing of the structural composite. But very importantly, it makes the electrochemical elements tolerant to mechanical deformations by preserving electrical contact of electrochemically-active elements. This feature is critical for continuous operation of batteries, for example, and indicates that the multifunctional materials approach used is a key enabler for the safe operation of structural energy-storing composites.





(c)

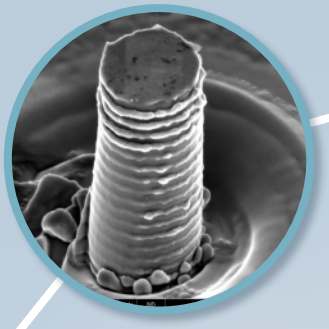


(d)

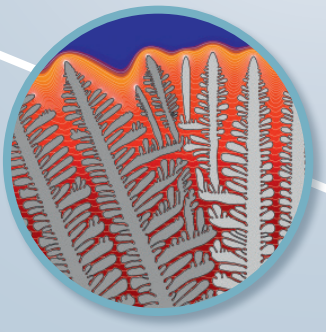
Figure 3: a) and b) Energy storage device made up with CNTF fabric as current collector, c) Resin infused glass fiber composite beams containing energy storage devices with and without shear connectors, d) Three-point bending of the beams containing energy storage devices.

[2] M. Rana, Y. Ou, C. Men, F. Sket, C. Gonzalez and J.J. Vilatela. *Damage-tolerant, laminated structural supercapacitor composites enabled by integration of carbon nanotube fibres.* **Multifunctional Materials 3**, 015001, 2020.

programme
Novel Alloy Design, Processing and Development



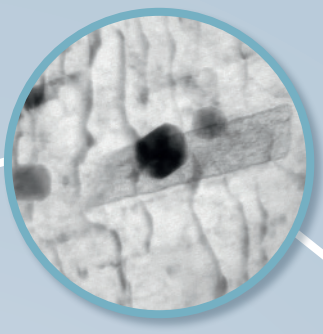
Nanomechanics



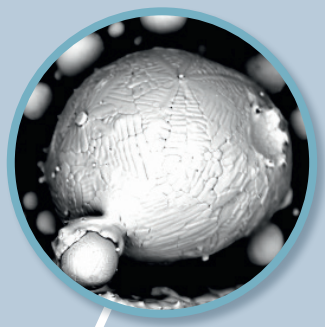
Modelling and Simulation of Materials Processing

Goal and vision

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

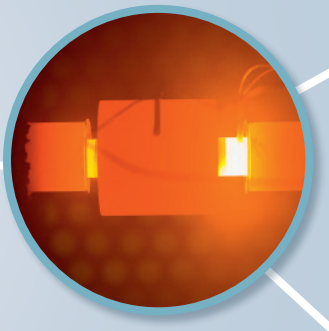


Physical Metallurgy

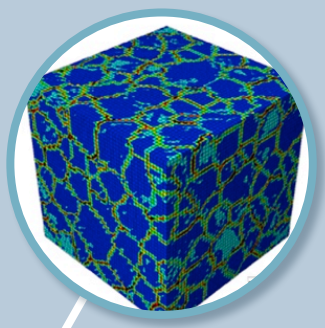


Solid State Processing

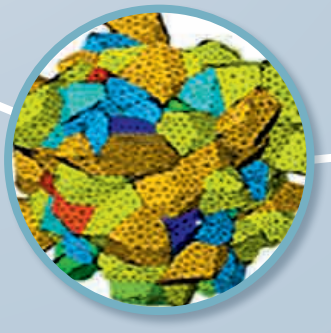
Solidification Processing and Engineering



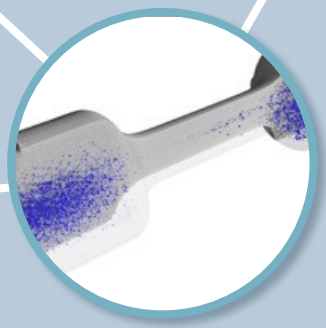
Physical Simulation



Mechanics of Materials



Multiscale Materials Modelling



X-Ray Characterisation of Materials

Main research lines

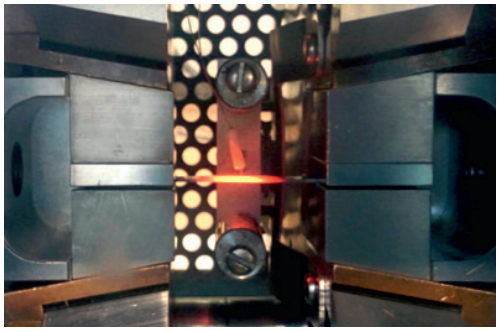
Main research lines

- **Characterisation** of microstructure and mechanical behaviour.
- **Advanced manufacturing:**
  - Solidification and casting.
  - Physical simulation of metallurgical processes (rolling, forging, extrusion, welding).
- **Powder metallurgy and additive manufacturing:**
  - Powder design and fabrication.
  - Process optimization.
- **Virtual processing:**
  Multi-scale modeling of solidification and phase transformations in metallurgical processing of metals and alloys.
- **Virtual testing:**
  Multi-scale modeling of the mechanical behavior of metallic polycrystals as function of their microstructure.

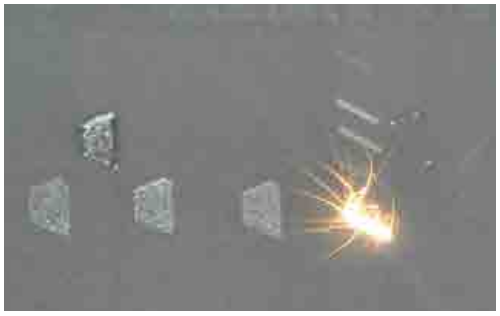
Materials of Interest

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

In-situ characterisation.



Thermo-mechanical processes in Gleeble thermo-mechanical simulator.



Advanced manufacturing.

Projects in focus

QPINOX / Development of new martensitic stainless steels for automotive lightweight structural applications

Funding: European Union, Research Fund for Coal and Steel (Grant Agreement 847195)
Partners: RINA Consulting – Centro Sviluppo Materiali SPA (Project Coordinator), IMDEA Materials Institute, Technische Universiteit Delft, ACERINOX EUROPE
Project period: 2019 - 2022
Principal Investigators: Dr. Ilchat Sabirov and Dr. Jon Molina

QPINOX project aims to generate a new class of affordable martensitic stainless steels for the automotive sector. It has two main objectives. First, to develop new martensitic stainless steel grades containing retained austenite, using a combination of quenching and partitioning process and steel chemistry optimisation, to achieve a unique combination of high tensile strength (> 1200 MPa) and ductility (> 15 %). This will be achieved by alloy and heat treatment design, first using models, and second via experiments, gradually scaling up from small heats with dilatometer heat treatment on small samples, to large heats followed by Gleeble heat treatment on larger hot rolled strips, and finally to lab pilot scale fully processed sheet production. The second main objective is to facilitate the industrial implementation of these new grades. It will be met by detailed experimental studies on critical automotive properties i.e. weldability, formability, fatigue, and corrosion. The project results are expected to benefit European stainless steel producers through the realisation of new and affordable martensitic stainless steel grades suitable for breakthrough into the lightweight automotive sector.

The main contribution of IMDEA Materials in the QPINOX project will be the development of the optimal heat treatments via physical simulation in GLEEBLE, analysis of microstructure, mechanical properties, fatigue properties and establishment of microstructure – property relationship in the developed steel grades.

Figure 1. Exit of the furnace for re-heating of slabs in hot rolling (courtesy of ACERINOX).

Figure 2. Slitting line (to make strips from the coil) for the final product (courtesy of ACERINOX).

CRACK TIAL / The high temperature fatigue behavior of a third generation gamma TiAl alloy for greener turbines

Funding: National Research Agency - Spanish Ministry of Economy, Industry and Competitiveness (MEIC) / National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges 2016
Partners: IMDEA Materials Institute
Project period: 2017 – 2019
Principal Investigators: Dr. Teresa Perez-Prado and Dr. Ilchat Sabirov

Enhancing transport sustainability is one of the great challenges of the XXI century. A reduction of at least 25% in fuel consumption and CO_2 emissions is ambitioned for the next generation of engines. Achieving this goal requires the integration of advanced materials and efficient designs. The successful incorporation into the intermediate pressure turbines (IPT) of lightweight 3rd generation titanium aluminides (TiAl), endowed with a better mechanical response at high temperatures and cyclic stresses than Ni-based superalloys, would contribute to dramatically improve efficiency under service conditions. However, the micromechanisms governing deformation and fracture of these materials are still unknown. The overarching aim of the CRACKTIAL project is to gain fundamental knowledge on the influence of microstructure, defects and temperature on the monotonic and fatigue response of a 3rd generation gamma-TiAl alloy within a wide temperature range. Phenomenological models linking these aspects will be built and will serve as guidelines for the design of more efficient, defect tolerant turbine components. This project is carried out in collaboration with ITP Aero.

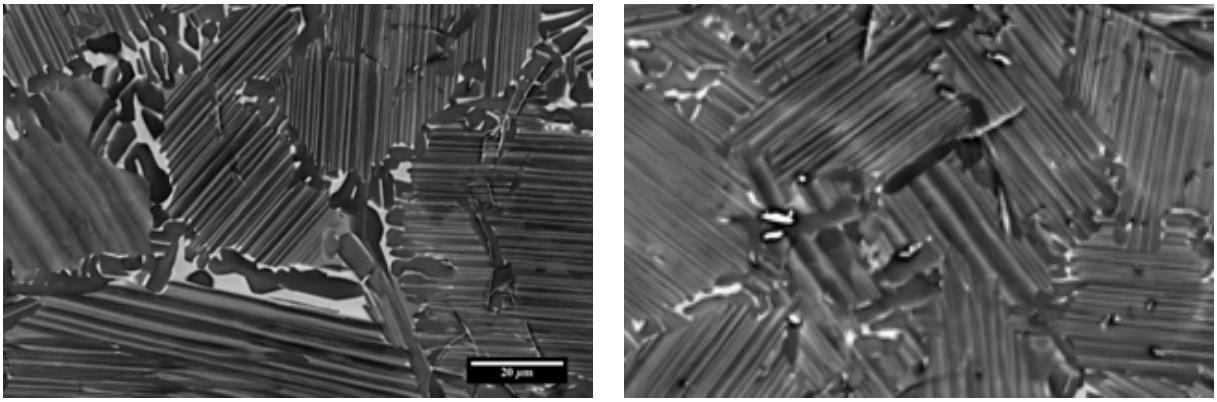
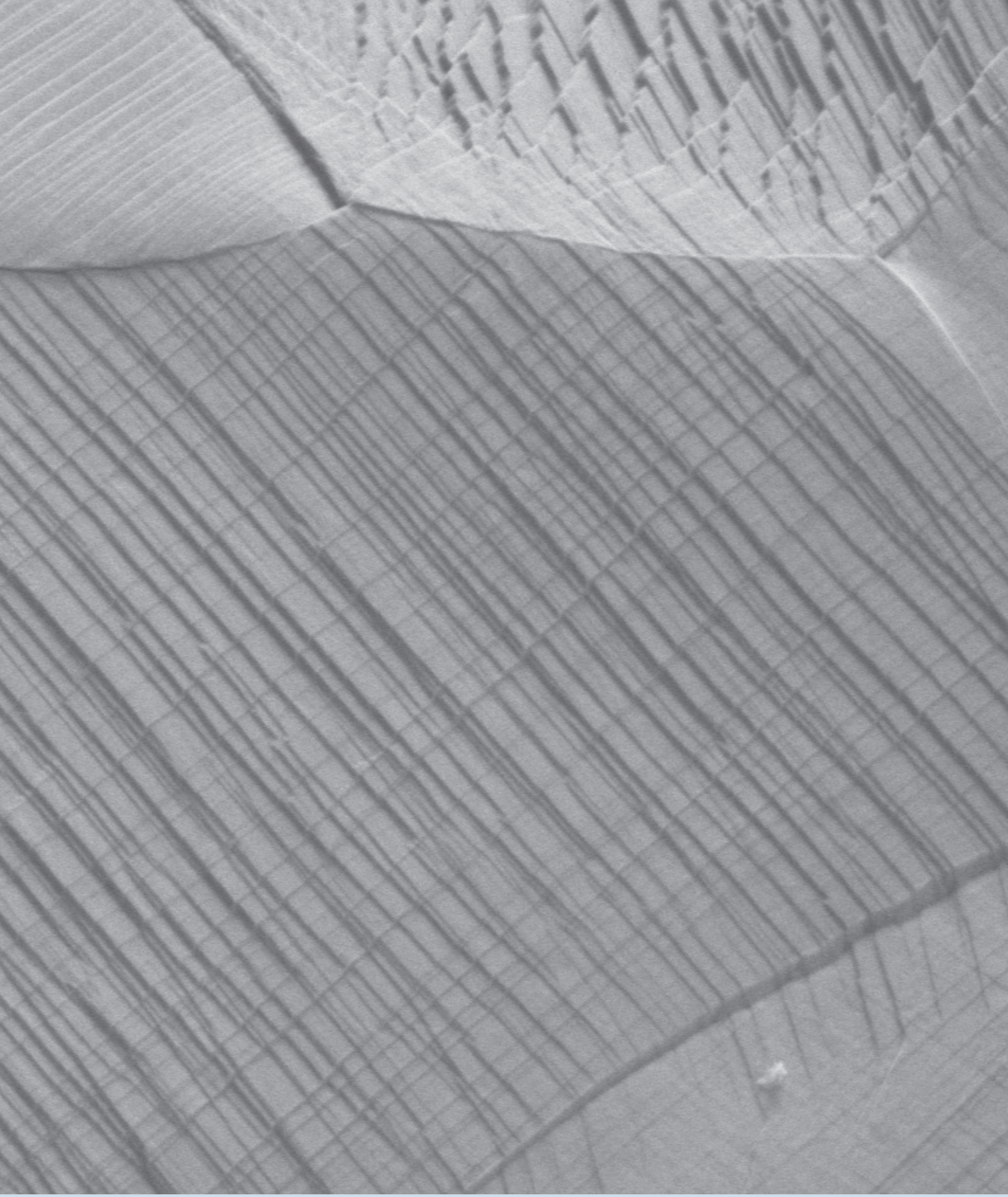


Figure 3. Representative microstructures of a cast 3rd generation gamma-TiAl alloy (Ti44Al4Nb1Mo0.7B) blade.



Scientific highlights

Development of porous Mg scaffolds for bone growth by additive manufacturing

Mg is a biocompatible and biodegradable metal with osteopromotive capabilities that is beginning to be used for bone repair and fixation in biomedical applications. Mg elastic modulus and density are closer to bone than those of other metallic alloys used in biomedical applications (stainless steel, Ti), limiting stress shielding effects. Moreover, the controlled degradation of Mg allows the progressive transfer of load to the new tissue and eliminates problems associated with the long term presence of metallic implants within the body.

Further biomedical applications of Mg are envisaged through the fabrication of porous Mg scaffolds for tissue engineering. In particular, selective laser melting of Mg alloys can be used to manufacture patient-specific porous scaffolds with geometries optimised for better mechanical support, osteoblast integration and vascularisation of the new tissue. Meotec GmbH and IMDEA Materials Institute are collaborating to fully optimize the microstructure of Mg scaffolds manufactured by this technique through the application of thermo-mechanical treatments, coatings and topology optimization strategies [1]. In particular, solution heat-treatments in combination with plasma electrolytic oxidation can be used to tailor the degradation resistance of the scaffolds in simulated body fluids so they can match tissue growth and provide enough mechanical strength during the whole healing process (Fig. 2). Moreover, finite element simulations of the scaffold can be used to assess the effect of degradation due to corrosion on the mechanical behavior to design patient-specific implants with optimum performance.

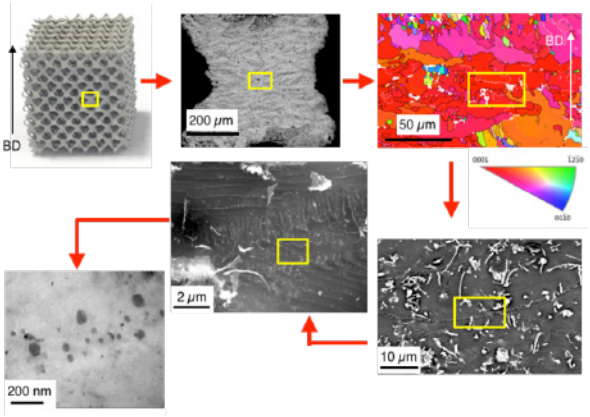


Figure 4. Microstructural analysis at different length scales of WE43 Mg alloy cubic porous scaffolds manufactured by selective laser melting. The dimensions of the scaffold at 10 x 10 x 10 mm3. BD stands for the building direction during selective laser melting.

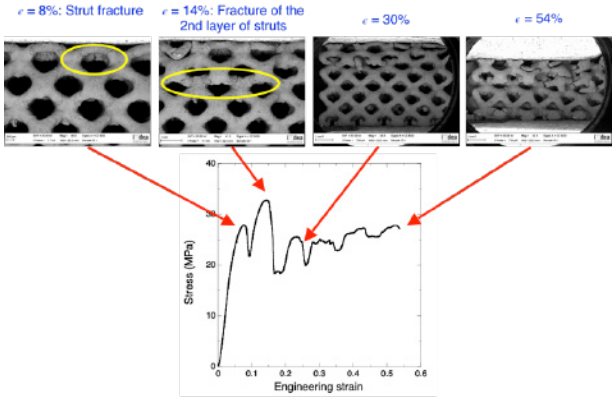


Figure 5. Mechanical test of the WE43 Mg porous scaffold within the scanning electron microscope showing the progress of damage during deformation.

Reference: [1] M. Li, T. Derra, A. Kopp, J. M. Molina-Aldareguía, J. LLorca. *Microstructure and mechanical properties of porous Mg scaffolds fabricated by additive manufacturing for biomedical applications.* **TMS 2020, 149th Annual Meeting and Exhibition**, San Diego, California, February 2020.

High throughput strategies applied to the discovery of new alloys

Magnesium has a large potential for more sustainable transport applications due to its low density. However, its poor strength and ductility limits its widespread application. The main fundamental problem arises from the low critical resolved shear stress (CRSS) for basal slip in Mg, which induces strain localization and early failure. Finding alloying strategies to strengthen basal slip in Mg alloys is critical, but conventional alloy design is costly and time consuming. In this work, a novel high-throughput methodology is used to measure the effect of alloying on the CRSS of basal slip in Mg alloys. The method is based on the combination of diffusion couples and micropillar compression, so that it avoids having to produce costly single-crystal specimens. Moreover, the method, applied to Mg-Zn and Mg-Al alloys, shows interesting solid-solution strengthening effects as a function of Zn and Al content.

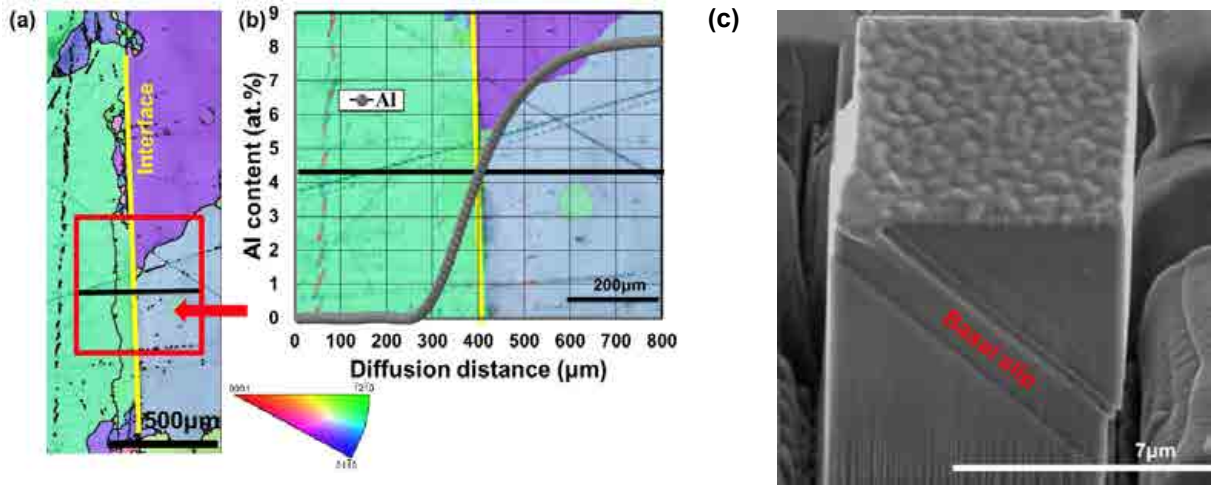


Figure 6. Interface area of diffusion couple showing (a) orientation, (b) Composition. By performing micropillar compression (c) along the black line, strengthening as a function of chemical content can be obtained

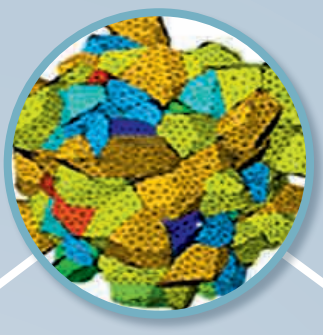
Reference: J-Y. Wang, N. Li, R. Alizadeh, M.A. Monclús, Y.W. Cui, J.M. Molina-Aldareguia, J. Llorca. **Acta Materialia 170**, 155-165, 2019.

programme
Integrated Computational Materials Engineering

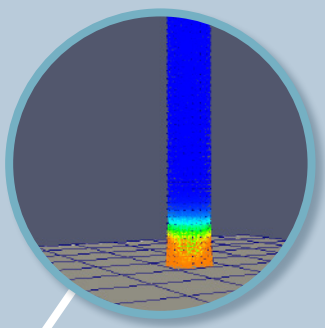
Goal and vision

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

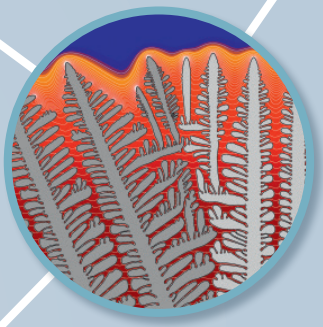
The expertise of the researchers in the programme covers a wide range of simulation techniques at different scales (electronic, atomistic, mesocopic and continuum) and is supported by a high performance computer cluster.



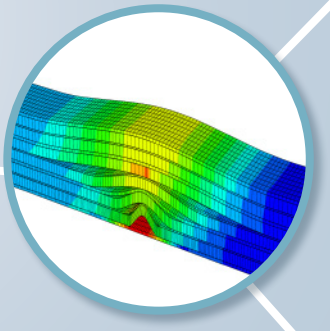
Multiscale Materials Modelling



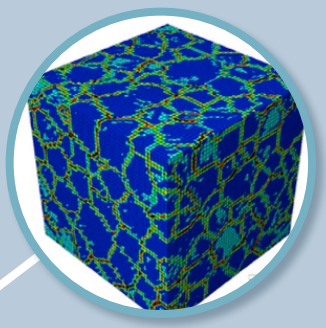
Computational Solid Mechanics



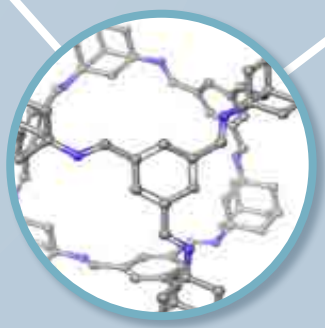
Modelling and Simulation of Materials Processing



Design & Simulation of Composite Structures



Mechanics of Materials



Computational and Data-Driven Materials Discovery

Main research lines

Virtual materials design, including virtual processing and virtual testing

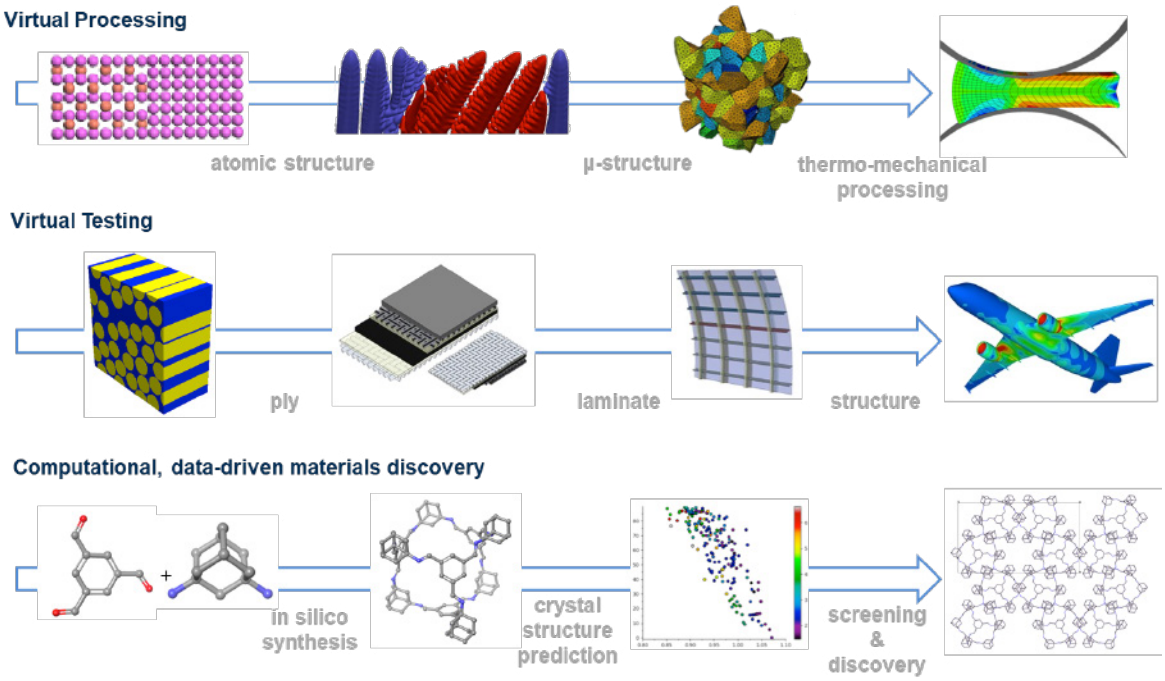
- Light (Al, Mg and Ti) metallic alloys and their composites. Ni-based superalloys. Multifunctional composite materials and structures. Materials for energy generation and storage.

Materials modelling at different length and time scales

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

Multiscale materials modelling

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



Projects in focus

MAFMA / Multiscale Analysis of Fatigue in Mg Alloys

Funding: European Union, Marie Skłodowska-Curie Individual Fellowship (Grant Agreement 795658)
Project period: 2019 – 2021
Principal Investigator: Dr. Anxin Ma
Supervisor: Prof. Javier LLorca

Magnesium and its alloys have attracted significant interest recently for engineering applications in automotive, aerospace, electronics, and biomedical sectors due to their low density, high specific-stiffness, superior damping capacity and biocompatibility. Nevertheless, these applications require a detailed knowledge of the deformation and failure mechanisms of Mg alloys, which are very complicated due to combination of different slip modes (basal, prismatic and pyramidal) together with twinning. They are fairly well-established under monotonic deformation but not in the case of cyclic loading.

The objective of the MAFMA project is to analyse the influence of twin formation and slip bands on the fatigue crack nucleation and growth of Mg alloys by means of multiscale models and *in situ* experiments. To this end, molecular dynamics, dislocation dynamics, phase field and crystal plasticity finite elements will be used to study twin nucleation and growth as well as the formation of persistent slip bands and the nucleation of fatigue cracks.

The initial activities of the project have been focussed in the development of a crystal plasticity model (including twinning and de-twinning) to predict the cyclic stress-strain curve of a Mg-1Mn-0.5Nd (wt.%). The representative volume element of the microstructure was built from the grain size distribution and the experimental pole figure (Fig. 1) and the experimental and simulated cyclic stress-strain curves are plotted in Fig. 2. The agreement between them was very good for different values of the applied cyclic strain semi-amplitude (0.8%, 2% and 4%). Moreover, the analysis of the micro-fields provided by the crystal plasticity finite elements simulations were used to formulate a fatigue indicator parameter.

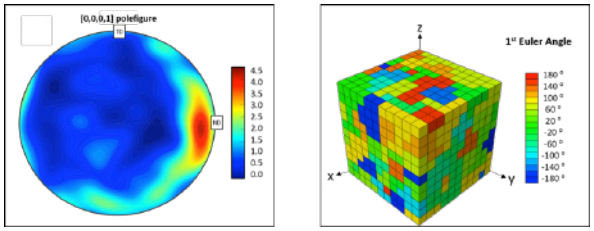


Figure 1. Experimental pole-figure, left plot, and representative volume element, right plot, of the microstructure of the Mg-1Mn-0.5Nd (wt.%) alloy used in the crystal plasticity simulations.

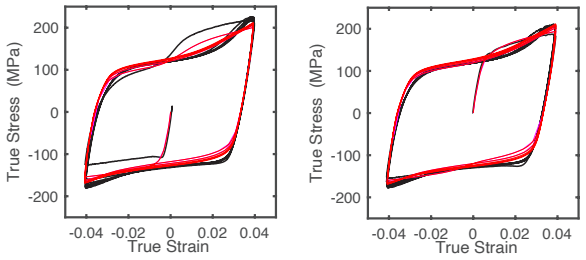


Figure 2. Experimental and simulated cyclic stress-strain curves of the Mg-1Mn-0.5Nd (wt.%) alloy subjected to a cyclic strain semi-amplitude of 4%. Experimental results are plotted as black lines, simulations are in red. The left curves correspond to specimens deformed initially in compression and the right one to initial deformation in tension.

CINEMA / Creating an Infrastructure for the Numerical Exploration of Metallurgical Alloys

Funding: Eurpean Commission, Horizon 2020 Programme, Marie Skłodowska-Curie Actions – Individual Fellowship (Grant Agreement 842795)
Project period: 2019 – 2021
Principal Investigator: Dr. Damien Tourret
Supervisor: Prof. Dr. Javier Segurado

The goal of the CINEMA project is to build a computational infrastructure for the exploration of metallurgical alloys and processing routes. It combines several state-of-the-art simulations methods in order to link solidification processing to microstructures and resulting mechanical properties. Computational thermodynamics (CalPhaD) is used to calculate phase diagrams of different alloys. Phase-field (PF) simulations provide the relation between a single dendrite tip morphology and its growth velocity. The PF simulations are then upscaled to hundreds or thousands of dendritic branches using a computationally-efficient multiscale solidification model in order to predict the microstructure, i.e. grain texture and dendritic structure, of a representative volume. This digital microstructure is then used in a crystal plasticity simulation to estimate its mechanical behavior and macroscopic homogenized properties. The completion of the project will set the foundations for computational discovery of structural metallic alloys by means of high throughput methods and machine learning. This will reduce the number of experiments required and thus substantial accelerate the development of new alloys and the optimization of processing routes.

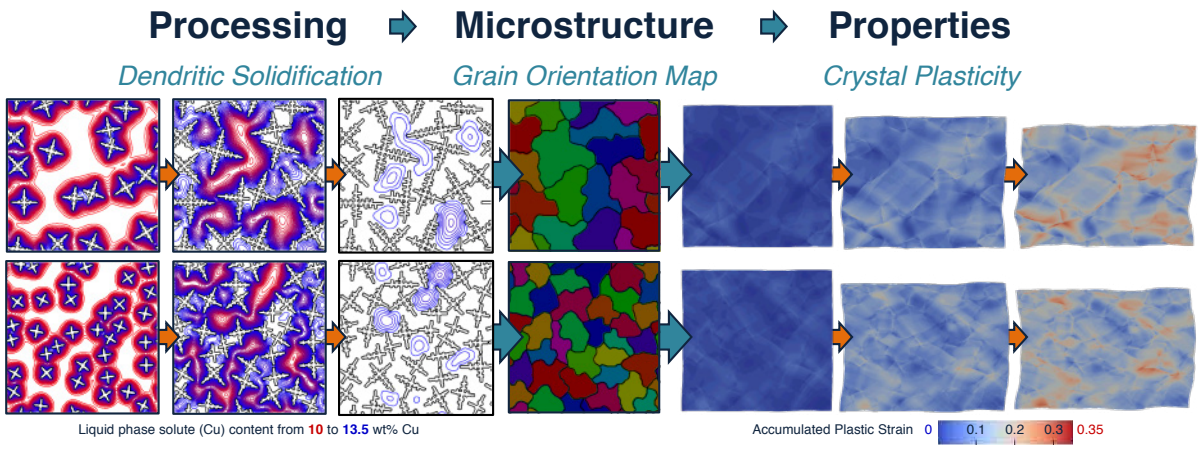
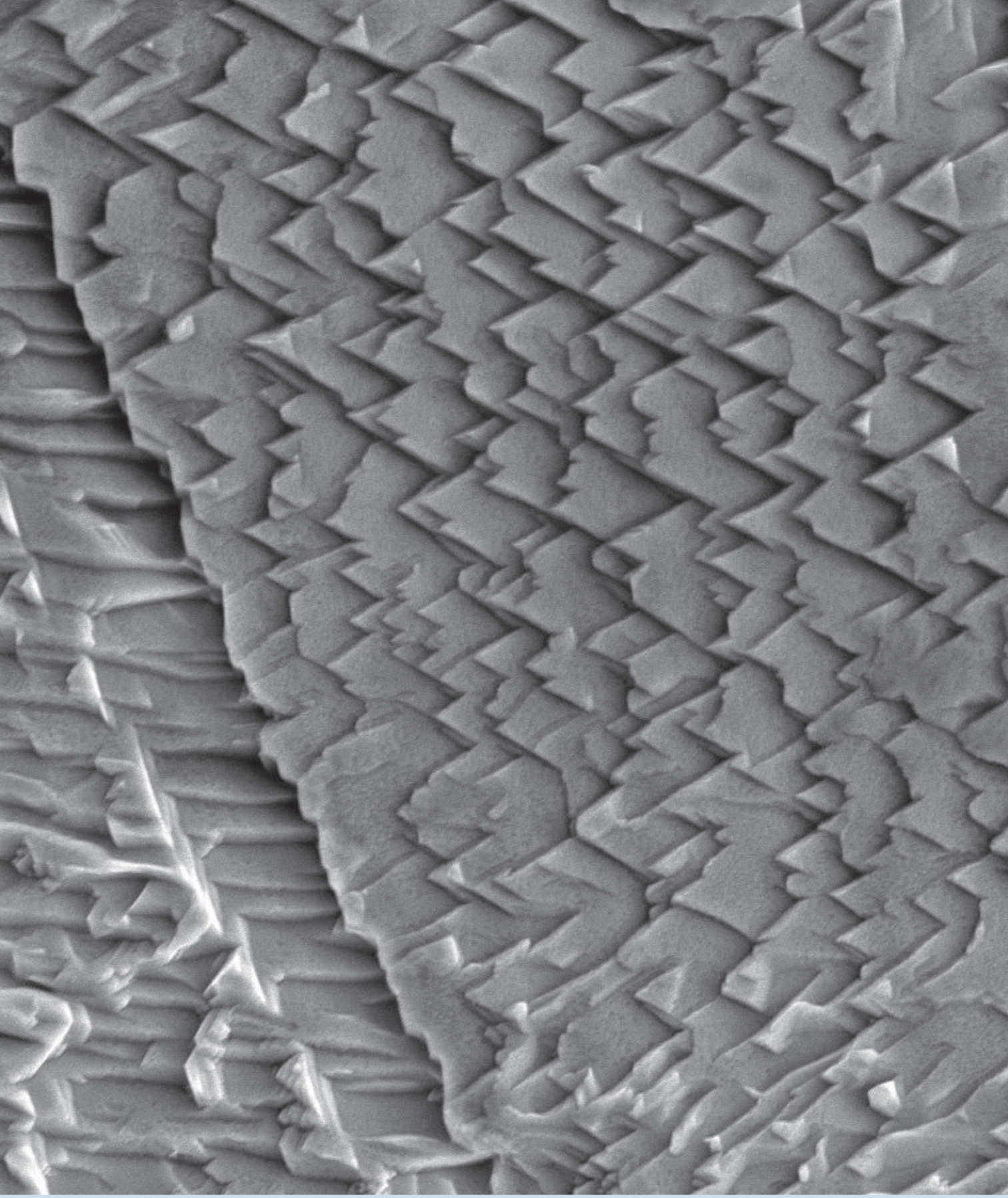


Figure 3. The CINEMA simulation framework combines multiscale simulations for dendritic growth and for crystal plasticity. Here, preliminary simulations show the solidification of an Al-10wt%Cu alloy undercooled by 10°C below its liquidus temperature (left) and mechanical loading of resulting heterogeneous microstructures up to 10% strain (right), for two different grain nucleation densities (top/bottom).



Scientific highlights

Simulation of multiphysical coupled problems in mechanics of materials

There are situations in which the mechanical response of a material is coupled with relevant physical phenomena occurring in parallel. Some examples are chemo-mechanical problems in which mechanical fields interact with the evolution of the local composition, as it happens during the deformation aided by mass diffusion, or thermo-mechanical coupled problems in which the temperature evolution is linked with the mechanical response and many more, as electro-mechanical, magneto-mechanical, etc. The mathematical models for the interaction of the processes involved in coupled problems is complex, and robust simulation techniques able to simulate the equations are fundamental to understand material behavior and improve the design under these conditions.

In IMDEA Materials Institute, a group of researchers has developed models and simulation techniques for these situations. As an example of this line, a thermo-mechanical coupled framework has been recently developed for metals, accounting for the effect of the polycrystalline microstructure [1]. In this framework, the metal is represented at the microscale considering explicitly the grains with their actual size, shape and orientations and the behavior of each grain is accounted for by the crystal plasticity model.

In each microscopic point, both the displacement and the temperature are considered as micro-field variables. The effect of temperature in the mechanical problem is the development of thermal strains and the change of material response due to the temperature dependency of the crystal plasticity model. On the other hand, plastic deformation by slip generates heat, so each point of the crystal might act as a heat source that has to be considered for the thermal problem. The numerical approach chosen to solve the problem is the finite method for both thermal and mechanical problems and a staggered strategy is used to account for the coupling effects. An example of this type of simulation is represented in Fig 4, showing the mechanical and thermal response of a Tantalum polycrystal, consisting of a representative volume element of its microstructure, deformed uniaxially at different strain rates.

This framework allows to study processes in which the thermomechanical coupling is fundamental, and microstructure plays an important role. An example is the simulation of the machining of a ferritic-perlitic steel considering its microstructure, composed by “soft” ferritic grains and “hard” perlite colonies. The results of these simulations are presented in Fig 5, and allow to analyze the effect of cutting speed, feed and material microstructure in the process performance.

References:

[1] J. Li, I. Romero, J. Segurado, Development of a thermo-mechanically coupled crystal plasticity modeling framework: Application to polycrystalline homogenization, International Journal of Plasticity 199, 313-330, 2019.

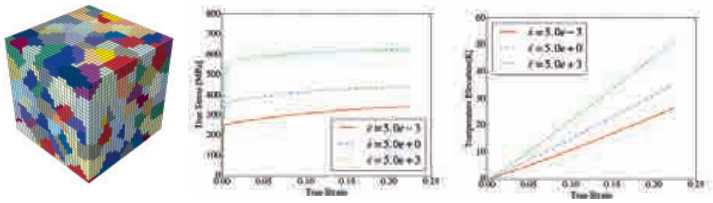


Figure 4. Effect of strain-rate in the deformation of Ta: Left, Representative Volume Element for the simulations. Center, stress-strain response. Right, average temperature evolution.

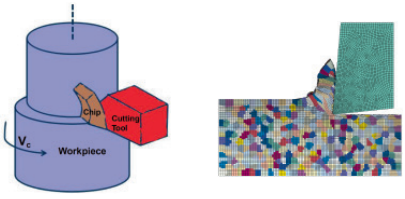


Figure 5. Thermo-mechanical Finite Element simulation of machining accounting for microstructure effect. Left, scheme of the process. Right, stage of the simulation during chip formation.

A microstructure and specimen size dependent fatigue modeling approach

The fatigue performance of a metallic alloy is strongly influenced by its microstructure, especially in the crack nucleation regime. Micromechanics based fatigue modeling [1] is the appropriate tool to account for this influence. In this framework, fatigue life is obtained from a fatigue indicator parameter (FIP), function of the microscopic field values (plastic strain, stress, etc) obtained by the numerical simulation of a Representative Volume Element (RVE) of the microstructure (Fig 6) subject to cyclic loading. The maximum *FIP* in a RVE determines its life (number of cycles *N*) through a phenomenological law calibrated with experiments (1)

$$N = \frac{FIP^{m}}{FIP_{c}} \quad (1)$$

in which FIP_c and m are the fitting parameters.

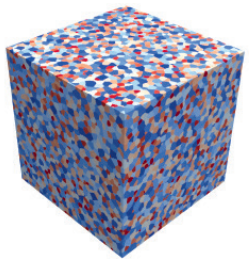


Figure 6. Representative Volume Element (RVE) of a polycrystal with 40.000 grains for FFT homogenization.

Although this framework has been successfully applied to predict fatigue life in many engineering alloys [1], it presents some limitations. Since fatigue life is triggered by the FIP value in the hottest point, the average life predicted is RVE size dependent and fatigue laws linking FIP with life are valid only for the particular RVE size used for calibration. Moreover, specimen or component size is not considered in the tool and the resulting predictions are not able to capture specimen size effects.

In IMDEA Materials Institute, a new *statistically based micromechanics fatigue modeling approach* has been proposed [2] in which the statistical distribution of FIPs in a macroscopic sample or component is obtained from the FFT simulation (using in this case the home-made code FFTMAD [3]) of a set RVEs of a relatively small size.

To this aim, first the cumulative probability distribution of the maximum FIP per RVE in a set of RVEs with size *V0*, CDF_0(FIP), is fitted to an extreme value distribution. Then, this distribution is extrapolated to the actual size of the specimen/component under study, *V1*, using the weakest link theory as

$$CDF_1(FIP) = CDF_0(FIP)^{V1/V0} \quad (2)$$

The life prediction law (eq. 1), now adjusted using two experiments and the CDF corresponding to the specimen size of those tests, is finally used to obtain the life distribution as function of the FIP distribution CDF_1. The life predictions of this new framework are RVE size independent and account for the effect of the specimen/component size. The result of this strategy is shown in Fig 7, where the methodology has been applied to an Inconel 718 alloy subjected to uniaxial strain controlled fatigue tests with different strain ranges $\Delta\varepsilon$.

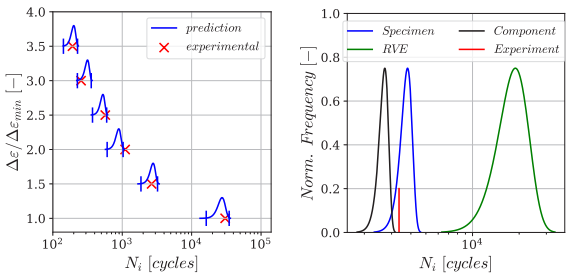


Figure 7. Left, life prediction (Number of cycles for initiation) as function of the applied cyclic strain range, $\Delta\varepsilon$. Right, life probability distribution for components of different sizes, small RVE size, typical specimen size and typical component size.

References:

[1] D. McDowell, F. Dunne. *Microstructure-sensitive computational modeling of fatigue crack formation.* **International Journal of Fatigue 32** (9), 1521-1542, 2010.

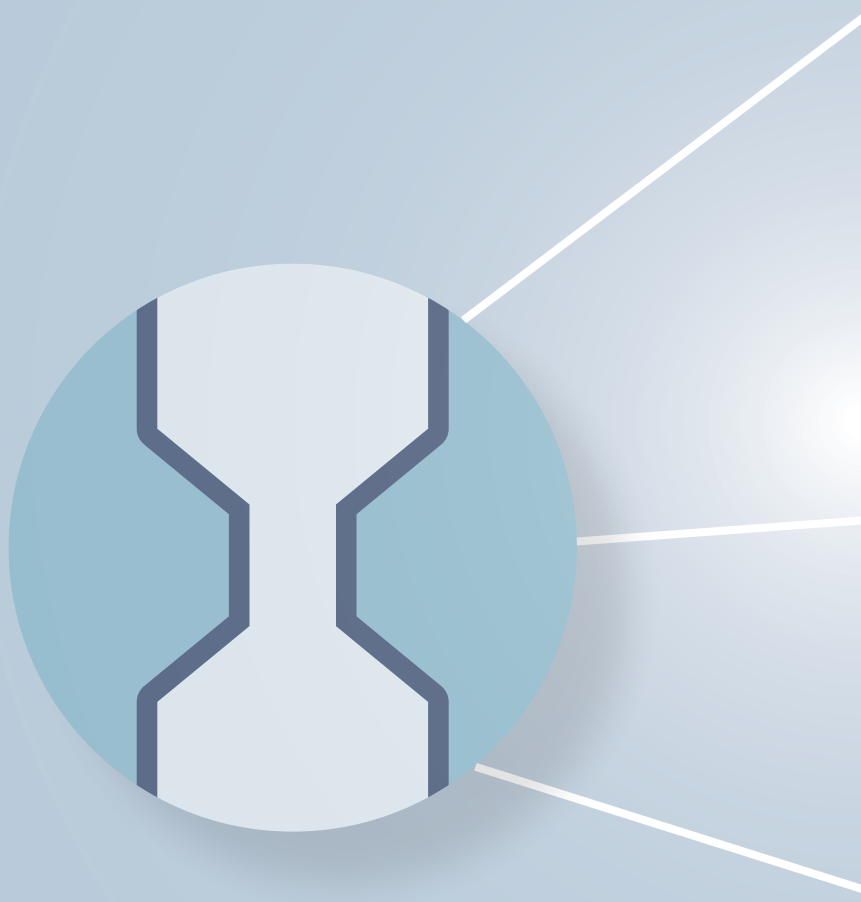
[2] S. Lucarini, J. Segurado. *An upscaling approach for micromechanics based fatigue: from RVEs to specimen and component life prediction*, **International Journal of Fracture**, doi:10.1007/s10704-019-00406-5, 2020.

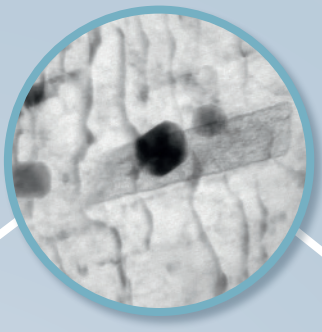
[3] S. Lucarini, J. Segurado. *On the accuracy of spectral solvers for micromechanics based fatigue modeling*", **Computational Mechanics 63** (2), 365-382, 2019.

programme
Multiscale Characterisation of Materials and Processes

Goal and vision

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



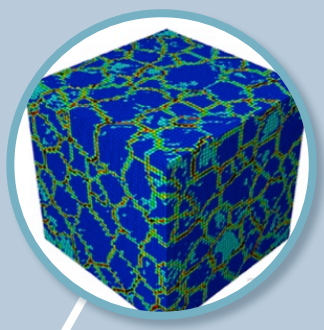


Physical Metallurgy

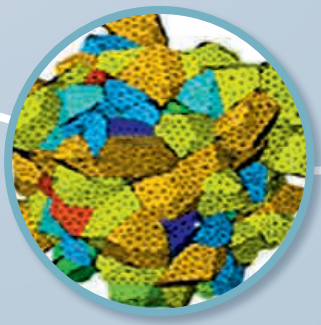
Multifunctional Nanocomposites

Nanomechanics

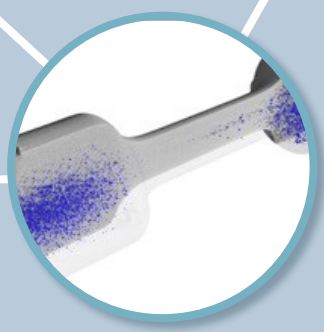
Structural Composites



Mechanics of Materials



Multiscale Materials Modelling



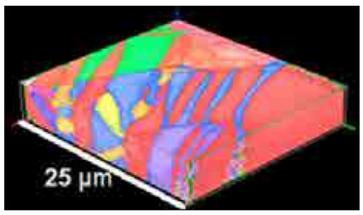
X-Ray Characterisation of Materials

Main research lines

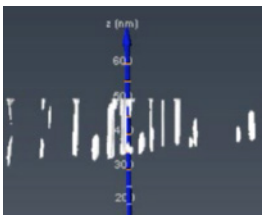
3D characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques:

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

XCT: Porosity in die-cast Mg alloys



3D-EBSD: Twin structure in a Mg alloy



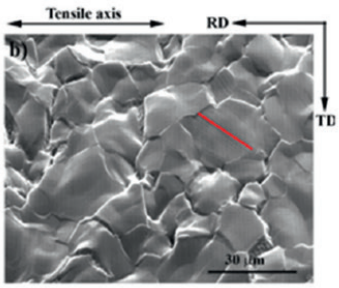
3D-TEM of Mg-Zn precipitates

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

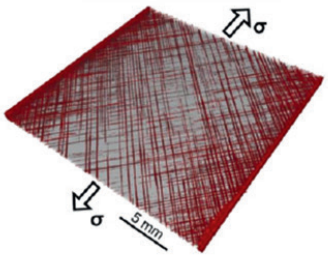
- **In-situ mechanical testing** across several length scales:
  - Tension, compression, fatigue, creep…of advanced metallic alloys and composites in the SEM and XCT.
  - Micro- and nanomechanical testing (nanoindentation, micropillar compression, microtensile testing…), including elevated temperature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

From mm....

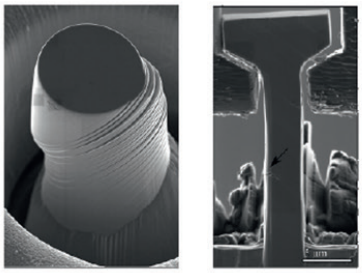
...to nm



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

MAT4.0-CM / Smart manufacturing of advanced materials for energy, transport and health

Comunidad de Madrid
EUROPEAN UNION
STRUCTURAL FUNDS

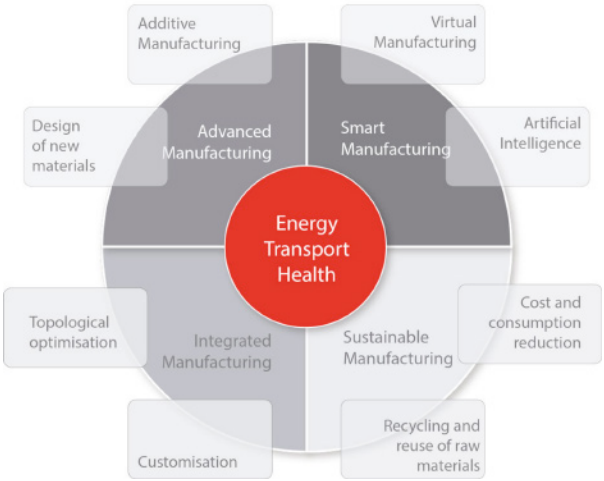
Funding: Regional Government of Madrid. Technologies 2018 (P2018/NMT-4381)
Partners: IMDEA Materials Institute (Coordinator), National Centre of Metallurgical Research (CENIM-CSIC), Carlos III University of Madrid (UC3M), Technical University of Madrid (UPM), Foundation for the Research Development and Application of composite materials (FIDAMC), Hospital La Paz Institute for Health Research (IdiPAZ)
Project period: 2019 – 2022
Principal Investigator: Dr. Jon Molina

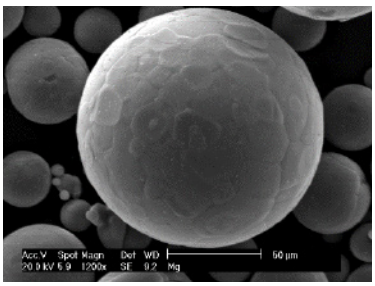
Research and innovation collaborative project involving key partners in the region of Madrid on the area of Smart Manufacturing of Advanced Materials with the long-term objectives of:

- Knowledge generation
- Implementation of advanced technologies in the productive sector
- Foster the creation of new innovative companies

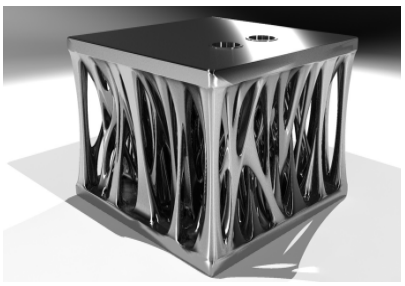
Ambitious short term fundamental research objectives in 6 areas:

- The design of new structural materials for 3D printing
- Understanding of process-microstructure-property relationships
- Topological optimization
- Use of advanced characterization techniques
- Development of online monitoring strategies
- Development of smart manufacturing strategies, combining online monitoring and advanced process simulation




Metallic powder particles


3D printing of metallic part


3D printed part

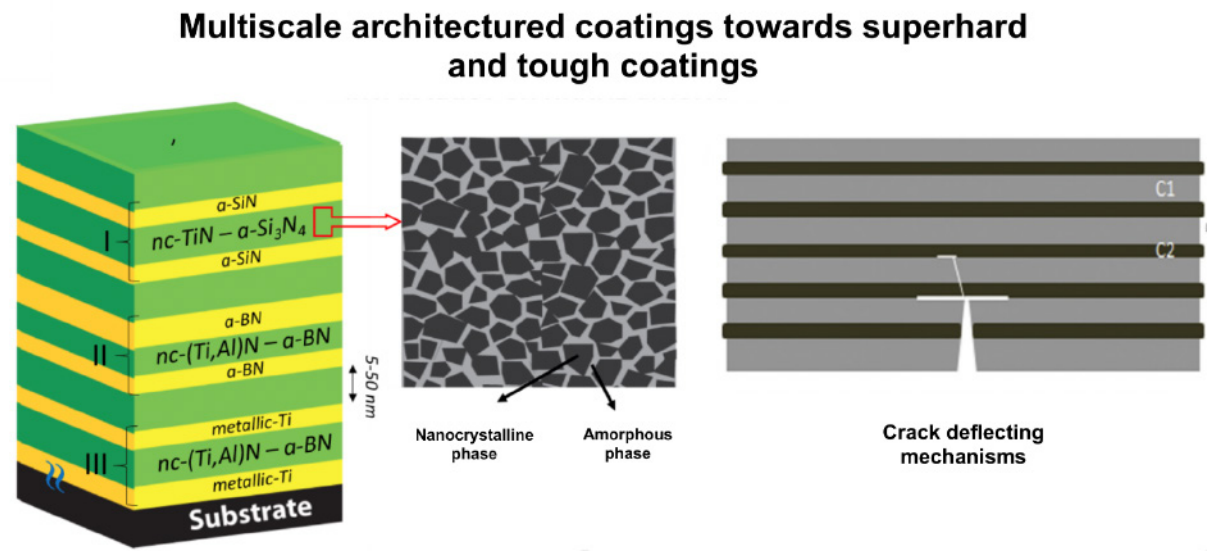
MULTIDUR / New generation of hard, tough and high temperature resistant multilayer coatings deposited by PVD / HiPIMS manufacturing

Funding: Regional Government of Madrid. Industrial Doctorate (IND2018/IND-9668)
Partners: Nano for Energy, S.L.U. and IMDEA Materials Institute
Project period: 2019 – 2022
PhD student: Álvaro Méndez
Supervisors: Dr. Jon Molina and Dr. Miguel Monclús

There is a growing demand from different industries for higher cutting speeds, feed rates and reduction in the use of lubricants during turning and milling operations. These higher performance requirements for different tools and cutting inserts used in multiple industrial applications require a new generation of advanced coatings that can resist increasing temperatures and withstand larger loads. Most of the hard coatings used to date are based on nitrides or carbides with monolithic structures (TiN, TiAlN, TiCN), mutilayers (TiAlN / TiN, TiN / TiB_2) or nanocomposites (nc-TiN / a-SiN) which exhibit in some cases very high hardness, and high resistance to temperature and oxidation. However, ceramic coatings tend to experience brittle failure due to their low fracture toughness.

Inspired by nature, MULTIDUR intends to combine the advanced concepts of nanocomposites and multilayers to increase the fracture resistance of hard coatings. The project will develop hard coatings based on multiscale architectures in the form of multilayers, alternating layers formed by Ti (Al, Si) N nanocomposites, consisting of TiN or (Ti, Al)N nanocrystals embedded in amorphous matrices (Si_3N_4 or BN) matrix, with dense and metastable amorphous layers (SiNx or BN), with individual layer thicknesses in between 5 and 50 nm.

These objectives will be achieved through a joint industrial doctorate between IMDEA Materials Institute and the company Nano for Energy, S.L.U., funded by the Comunidad de Madrid.



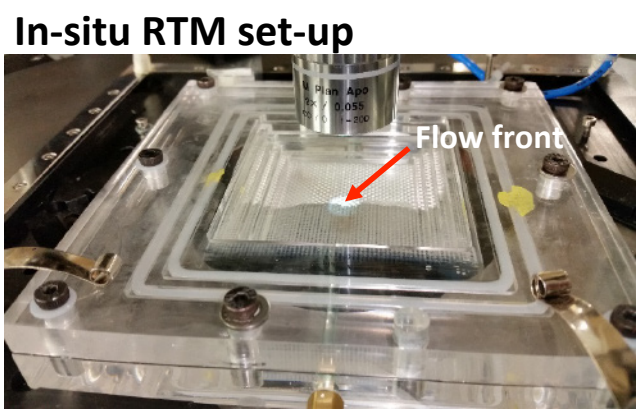
Philosophy behind the MULTIDUR project

Multiscale Characterisation of Materials and Processes

Scientific highlights

In-situ XCT infiltration of fibers by resin transfer molding process

Fibre-reinforced polymers are extensively used in the automotive, aerospace and energy industries for structural applications. The interest in Liquid Composite Molding (LCM) processes, for the production of composite materials has grown in the last years, especially in the vacuum assisted resin transfer moulding (VARTM) process due to its relative low cost and the possibility to process large panels, for example for wind turbine blades. Fibre infiltration during XCT measurements, allows to investigate the infiltration process and characterize the formation and transport of pores in the process in 4D. Several parameters such as resin velocity, resin viscosity, application of vacuum pressure, the dual scale flow behavior and its effect on the microstructure can be accurately studied by these in-situ XCT measurements. The figure below shows the set-up of the experiment developed at IMDEA for laminography experiments and fast-tomography experiments.



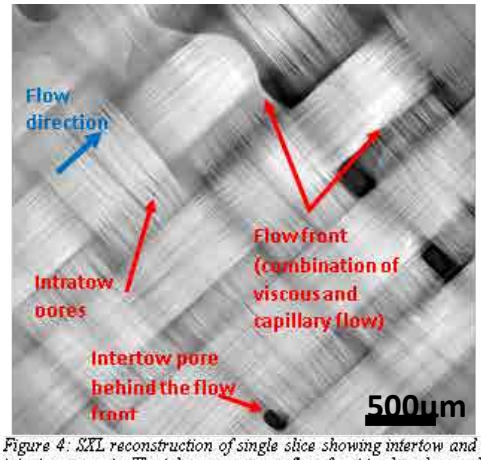


Figure 4: SXL reconstruction of single slice showing intertow and intratow porosiy. The inhomogeneous flow front is also observed.

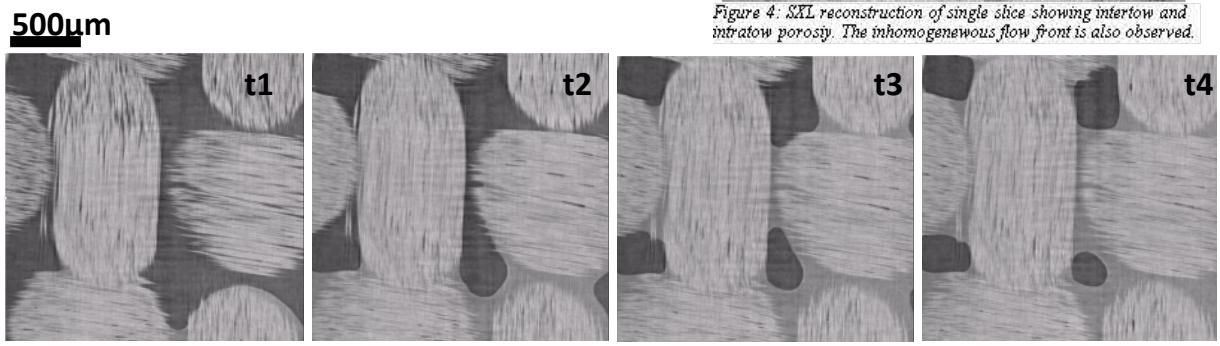


FIgure1. Time sequence as obtained from XCT in the same slice in-situ RTM

Mechanical behavior of InP twinning superlattice nanowires

It has been shown that InP semiconductor nanowires carry charge and excitons efficiently and also exhibit very high optical efficiency. Their mechanical properties are extremely important, as mechanical strain strongly influences the electric, optical and magnetic properties. However, this information is very limited due to the difficulties associated with the mechanical testing of nanowires. In this work, the mechanical properties and fracture mechanisms of individual InP TSL nanowires in tension were ascertained by means of in situ uniaxial tensile tests in a transmission electron microscope. The elastic modulus, failure strain, and tensile strength along the [111] direction were determined. No evidence of inelastic deformation mechanisms was found before fracture, which took place in a brittle manner along the twin boundary. Moreover, a good agreement with the results of Molecular Dynamic Simulations was obtained.

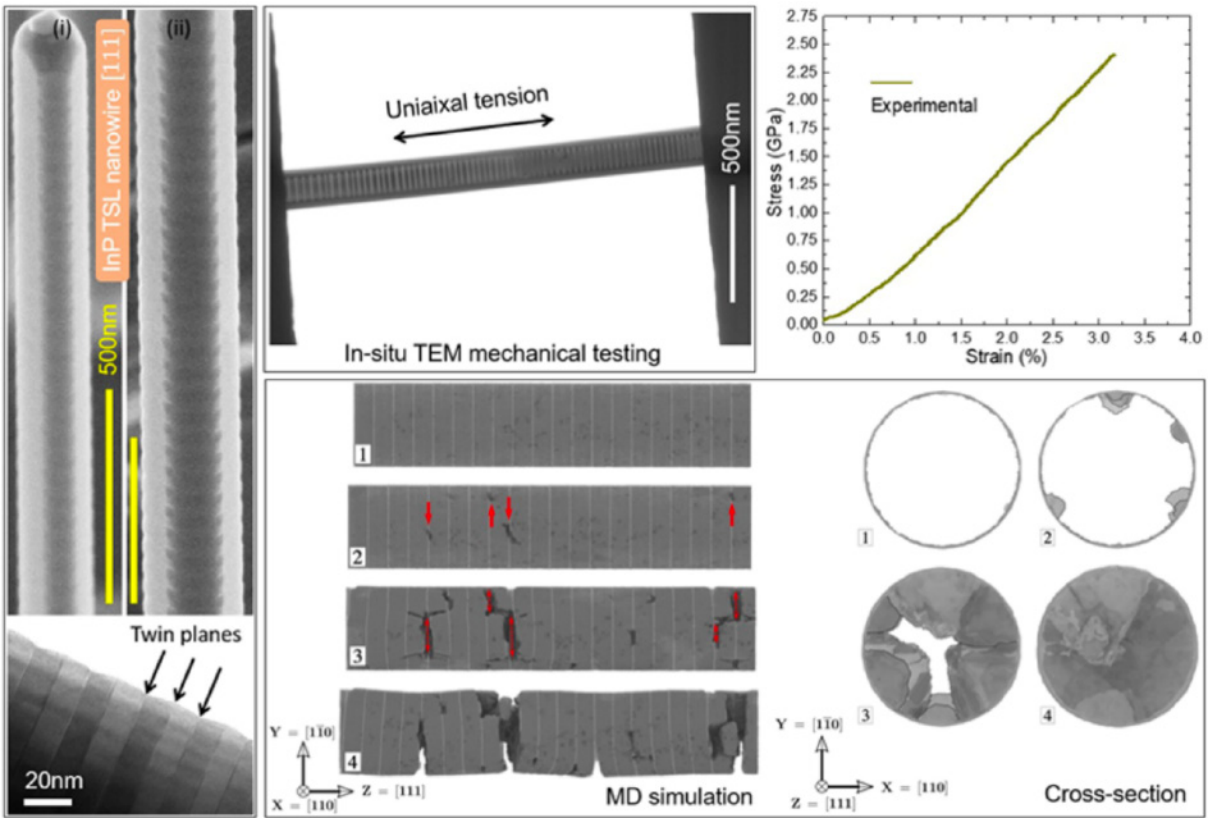


Figure 2.

References:

Z. Liu, I. Papadimitiriou, M. Castillo-Rodríguez, C. Wang, G. Esteban-Manzanares, X. Yuan, H.H. Tan, J.M. Molina-Aldareguia, J. LLorca. **Nano Letters 19**, 4490-4497, 2019.

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.

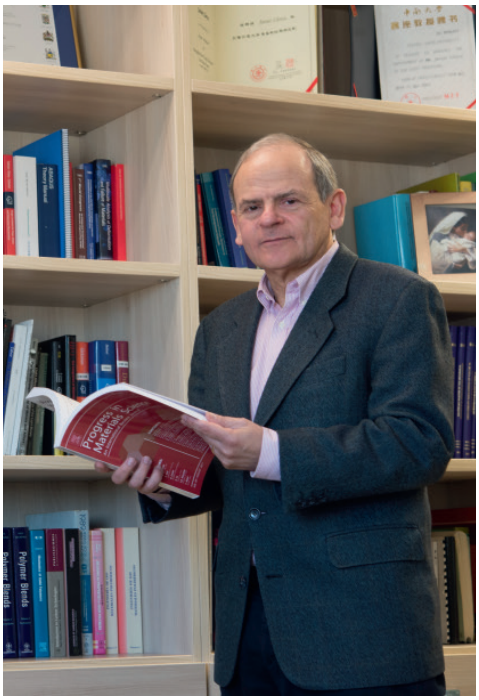
Dr. María Teresa Pérez-Prado

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

Dr. Jon M. Molina-Aldareguía

Senior Researcher, Micromechanics and Nanomechanics

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

Research Interests

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

Dr. Javier Segurado

Senior Researcher, Multiscale Materials Modelling

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

Associate Professor of Materials Science, Technical University of Madrid

Research Interests

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

Dr. Juan José Vilatela

Senior Researcher, Multifunctional Nanocomposites

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

Research Interests

Development of macroscopic materials made up of nanobuilding blocks in a way that the unique properties at the nanoscale are preserved through the assembly process and a new generation of 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.

Dr. Cláudio Saul Lopes

Senior Researcher, Design & Simulation of Composite Structures

Ph.D. in Aerospace Engineering from Delft University of Technology. The Netherlands

Research Interests

Design and simulation of composite materials and structures; multiscale computational analysis of composites; damage and failure of composite materials; impact and damage tolerance of composite structures; non-conventional multiscale composite design and manufacturing; additive manufacturing of composites; recycling of composite materials.

Dr. De-Yi Wang

Senior Researcher, High Performance Nanocomposites

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

Research Interests

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

Dr. Srdjan Milenkovic

Senior Researcher, Solidification Processing & Engineering

Ph.D. in Materials Engineering from State University of Campinas. Brazil

Research Interests

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

Dr. Maciej Haranczyk

Senior Researcher, Computational and Data-Driven Materials Discovery

Ph.D. in Chemistry from University of Gdansk. Poland

Research Interests

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

Dr. Ilchat Sabirov

Senior Researcher, Physical Simulation

Ph.D. in Metallurgy from Montanuniversitaet Leoben. Austria

Research Interests

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

Dr. Ruben D. Costa

Senior Researcher, Hybrid Optoelectronic Materials and Devices

Ph.D. in Chemistry from the University of Valencia. Spain

Research Interests

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

Researchers

Dr. Federico Sket

Researcher, X-ray Characterisation of Materials

Ph.D. in Materials Engineering from Max-Planck Institute for Iron Research. Germany

Research Interests

Microstructural evolution of metal alloys and fibre-reinforced composites for engineering applications using advanced laboratory and synchrotron X-ray tomography as well as X-ray diffraction; processing of composite materials and relationship between processing conditions and microstructural evolution; mechanical deformation of materials and evolution of mechanical and microstructural properties; development of in situ devices (based on in-situ X-ray microtomography and X-ray diffraction) for testing mechanical properties and processing using X-rays; and incorporation of experimental results to the development of physically-based models for optimisation of material processing and properties.

Dr. Damien Tourret

Researcher, Modelling and Simulation of Materials Processing

Ph.D. in Materials Science and Engineering from Mines ParisTech, France

Research Interests

Microstructure selection, formation, and evolution; solidification processing (e.g. casting, welding, additive manufacturing); structural materials; metals and alloys; crystal growth; phase transformations; multiscale modelling; phase-field modelling; parallel computing (e.g. using graphics processing units); 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

Prof. José Manuel Torralba
Visiting Scientist

Ph.D. in Metallurgical Engineering in Technical University of Madrid

Professor of Material Science and Engineering in Carlos III University of Madrid, Spain

Research Interests
His main scientific-technical field of interest is Powder Metallurgy, Physical Metallurgy, Advanced consolidation methods (SPS, MIM, SLM,...) and powder production methods (atomizing, mechanical alloying). Design and develop of new alloys and materials such as metal matrix composites, superalloys, steels, high entropy alloys and intermetallics.

Dr. Álvaro Ridruejo
Visiting Scientist

Ph.D. in Material Science in Technical University of Madrid

Associate professor of Material Science in Technical University of Madrid, Spain

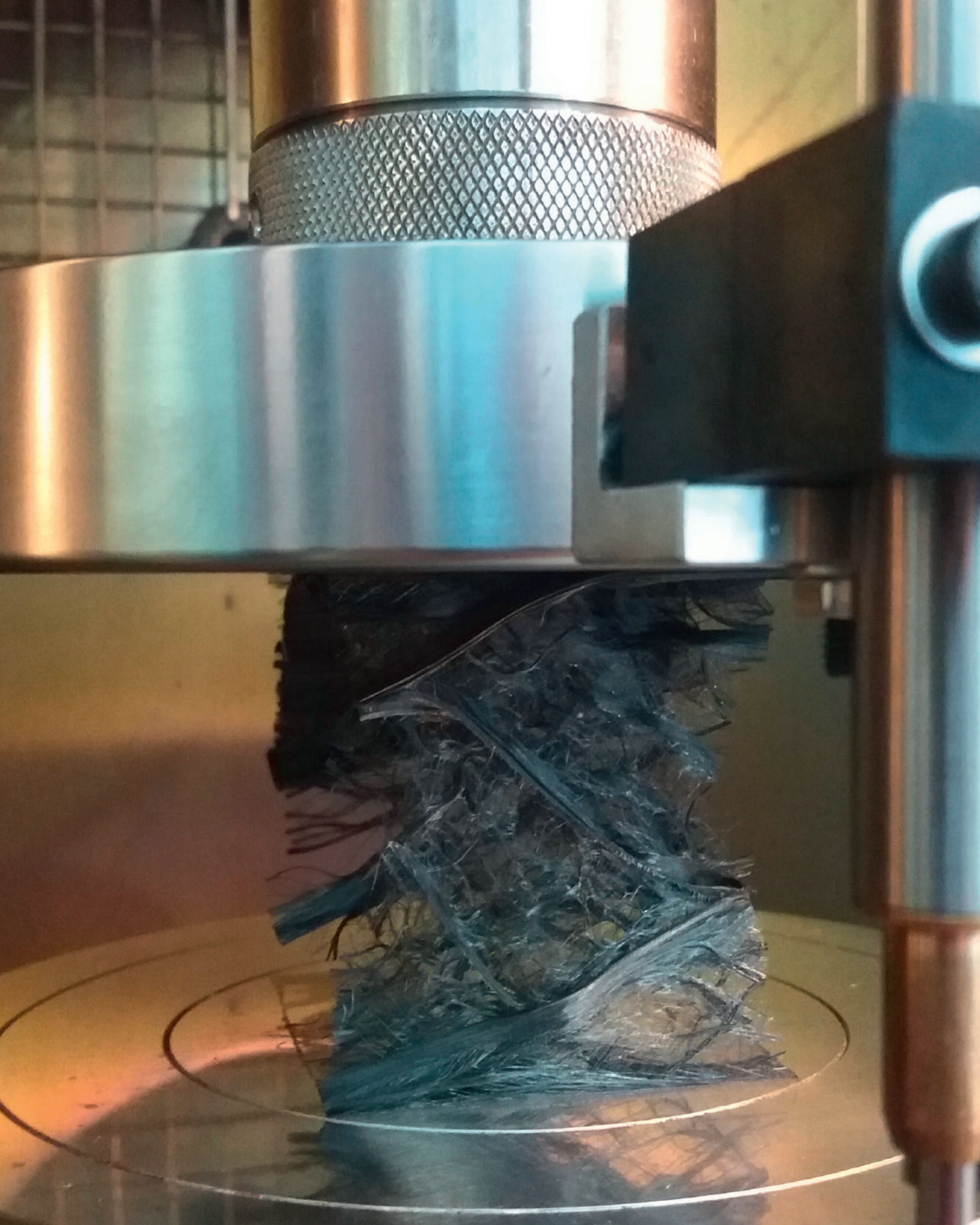
Research Interests
His main interest is the relationship between structure and properties in a broad sense. In particular, he is now collaborating with the MNG group in the study of the mechanical properties of CNT-based fibrous materials by means of advanced characterization methods and multiscale modelling of fibre networks, and with the Structural Composites group in the development of new thermoplastic matrix composites.

Prof. Wen Zhang
Visiting Scientist

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

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

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



annex

1. R&D projects and contracts

1.1. European R&D Projects (European Commission)

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. Ilchat Sabirov and Dr. Jon Molina

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. Jianfang Cui; Supervisor: Dr. De-Yi 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. Anxin Ma; Supervisor: Prof. Javier LLorca

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. Damien Tourret; Supervisor: Dr. Javier Segurado

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

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

Title/Acronym: Nanostructured yarn composites for structural energy storage/ENERYARN
Partners: IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - IF
Principal Investigator: Dr. Anastasiia Mikhalchan; Supervisor: Dr. Juan José Vilatela

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

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

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

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

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. Juan José Vilatela

Title/Acronym: CROR engine debris impact shielding. Design, manufacturing, simulation and impact test preparation/REDISH
Partners: IMDEA Materials Institute (Coordinator), Foundation for Research Development and Application of Composite Materials (FIDAMC)
Period: 2016 – 2019
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Clean Sky Joint Undertaking 2
Principal Investigator: Dr. Cláudio S. Lopes

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

Title/Acronym: A novel process for manufacturing complex shaped Fe-Al intermetallic parts resistant to extreme environments/EQUINOX
Partners: National Technical University of Athens (Coordinator), Elastotec GmbH Elastomertechniken, Kochanek Entwicklungsgesellschaft, Technica Univerzita V Liberci, Access e.V., Open Source Management Limited, CES Operations AS, Freni BREMBO Spa, Yunzhnoye Design Office named after Mikhail Yangel, IMDEA Materials Institute
Period: 2016 – 2019
Funding Institution/Programme: European Commission/Horizon 2020 Programme – SC5
Principal Investigators: Dr. Srdjan Milenkovic and Dr. Federico Sket

Title/Acronym: Dynamic behaviour of composite materials for next generation aeroengines/DYNACOMP
Partners: IMDEA Materials Institute (Coordinator), HEXCEL Composites, Micro Materials Ltd., Technical University of Madrid, Madri+d foundation
Period: 2016 – 2020
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - ITN - EID
Principal Investigators: Dr. Jon M. Molina, Prof. Carlos González and Dr. Federico Sket

Title/Acronym: Multi-functional nano-carbon composite materials network/MULTICOMP
Partners: Multiple partners coordinated by the Karlsruhe Institute of Technology (Coordinator)
Period: 2016 – 2020
Funding Institution/Programme: European Commission/Horizon 2020 Programme – COST Actions
Principal Investigator: Dr. Juan Pedro Fernández

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

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1.2. Other International R&D Projects

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 Investigators: Dr. Claudio Lopes and Prof. Carlos González

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

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

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 2018
Principal Investigator: Prof. Javier LLorca

Title/Acronym: Engineering nanoparticle electron transfer in hybrid dye-metal oxide semiconducting materials for low temperature solar cells/HyNanoSC
Partners: University of Alicante (Coordinator), IMDEA Materials Institute
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 2018
Principal Investigator: Dr. Rubén Costa

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 2018
Principal Investigator: Dr. Claudio Lopes

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 2018
Principal Investigator: Dr. Damien Tourret

Title/Acronym: Field Emission Scanning Electron Microscope for materials characterisation with EDX and EBSD
Partners: IMDEA Materials Institute
Period: 2019 – 2020
Funding Institution/Programme: Spanish Ministry of Science, Innovation and Universities (MCIU)/Scientific and Technical Infrastructure and Equipment 2019
Principal Investigator: Dr. Jon Molina

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 2018
Coordinator: Miguel Ángel Rodiel

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 2017
Principal Investigator: Dr. Vinodkumar Etacheri

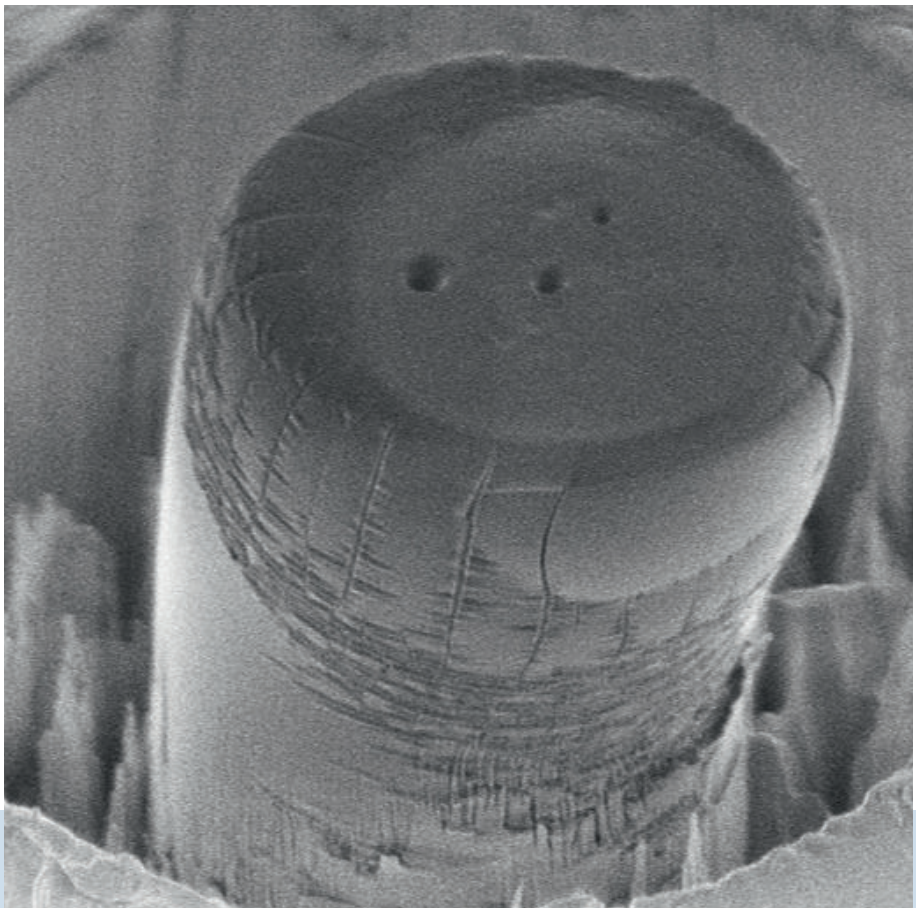
Title/Acronym: Virtual environment for the design and manufacturing of airplane turbine engines/ENVIDIA
Partners: ITP Aero (Coordinator), Technical University of Madrid, University of País Vasco, IMDEA Materials Institute
Period: 2018 – 2020
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy and Competitiveness (MINECO)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Collaboration Challenges 2017
Principal Investigator: Dr. Damien Tourret

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

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

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

Title/Acronym: The high temperature fatigue behavior of a third generation gamma TiAl alloy for greener turbines/CRACK-TIAL
Partners: IMDEA Materials Institute
Period: 2017 – 2019
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy, Industry and Competitiveness (MEIC)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges 2016
Principal Investigators: Dr. Teresa Pérez-Prado and Dr. Ilchat Sabirov



Title/Acronym: Ultrafine eutectics by laser additive manufacturing/ELAM
Partners: German Aerospace Research Center (Coordinator), Access e.V., Wigner Research Centre for Physics, Fraunhofer Institute for Laser Technology, Bosch-Mahle Turbosystems GmbH, P&G Manufacturing GmbH, IMDEA Materials Institute
Period: 2017 – 2020
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy, Industry and Competitiveness (MEIC) - European Commission/Horizon 2020 Programme – M-ERA.NET 2/International Joint Actions 2017
Principal Investigator: Dr. Federico Sket

Title/Acronym: Fiber metal laminates for application in marine renewable energy/ACERCOM
Partners: ArcelorMittal (Coordinator), Technical University of Madrid, IMDEA Materials Institute
Period: 2016 – 2019
Funding Institution/Programme: National Research Agency - Spanish Ministry of Economy and Competitiveness (MINECO)/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Collaboration Challenges 2016
Principal Investigator: Prof. Carlos González

1.4. Regional R&D Projects

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 (UC3M), Technical University of Madrid (UPM), Foundation for the Research Development and Application of composite materials (FIDAMC), Hospital La Paz Institute for Health Research (IdiPAZ)
Period: 2019 – 2023
Funding Institution/Programme: Regional Government of Madrid/Technologies 2018
Principal Investigator: Dr. Jon Molina

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 2018
Principal Investigator: Dr. Juan José Vilatela

Title/Acronym: Advanced manufacturing technologies for the new generation of composite materials/TEMACON
Partners: Airbus Operations (Coordinator), Zinkcloud, Obuu Tech, Foundation for the Research Development and Application of composite materials (FIDAMC), IMDEA Materials Institute
Period: 2019 – 2022
Funding Institution/Programme: Regional Government of Madrid/Open Innovation Hubs
Principal Investigator: Prof. Carlos 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. Jon Molina and Dr. Miguel 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. Maciej Haranczyk

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

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

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

Title/Acronym: The next generation of rechargeable Li-O_2 batteries
Partners: IMDEA Materials Institute
Period: 2017 – 2021
Funding Institution/Programme: Regional Government of Madrid/Grant for research talent atraction. Modality 1
Principal Investigator: Dr. Vinodkumar Etacheri

1.5. Privately-funded R&D Projects

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

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

Title/Acronym: Study on new technique to anti-shrinking PPS fiber at ignition and during burning/PPS
Company: Sichuan Unfire Polymer Material Technology
Period: 2019
Principal Investigator: Dr. De-Yi Wang

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

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

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

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

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

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

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

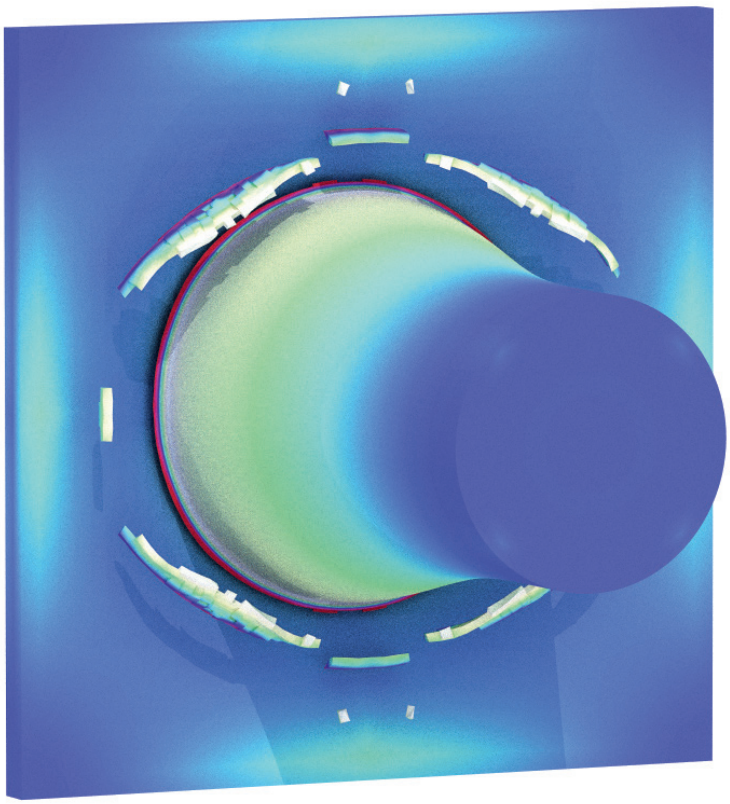
Title/Acronym: Development of batteries on flexible plastic substrates/BATFLEX
Company: Grupo Antolin
Scientific Partner: IMDEA Energy
Period: 2018 - 2020
Principal Investigator: Dr. Juan José Vilatela and Dr. Rebeca Marcilla

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

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

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

Title/Acronym: Functionalization of natural brucite and its application in polymers/ TOBEST
Company: Liaoning Jinghua New Materials
Period: 2018-2019
Principal Investigator: Dr. De-Yi Wang



Title/Acronym: Alloy design for additive manufacturing of steels
Company: Metal sector
Period: 2018-2019
Principal Investigator: Dr. Damien Tourret

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

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

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

1.6. Licenses

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

2. Fellowships

2.1. International

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Programme: Juan de la Cierva
Period: 2017-2019
Funding Institution: Spanish Ministry of Economy and Competitiveness
Dr. A. Baluch

Programme: Juan de la Cierva
Period: 2017-2019
Funding Institution: Spanish Ministry of Economy and Competitiveness
Dr. V. Etacheri

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

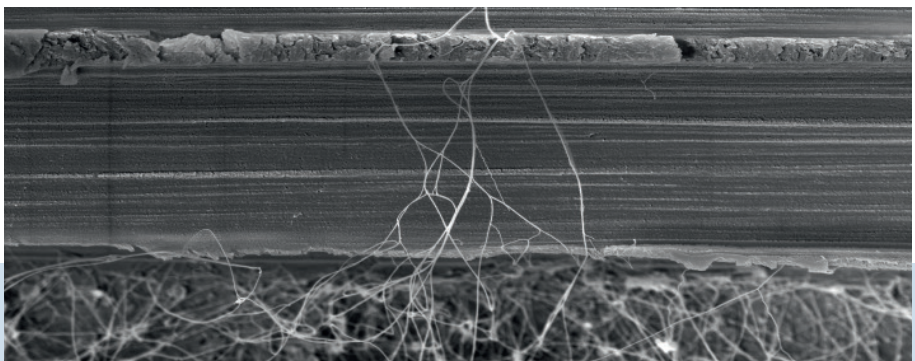
Programme: Training University Lecturers (FPU)
Period: 2018-2021
Funding Institution: Spanish Ministry of Education, Culture and Sport
R. Santos

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: 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: 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. Malik

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 2
Period: 2019-2023
Funding Institution: Madrid Regional Government
Dr. S. Liu

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

Programme: Talent Attraction Programme – Modality 2
Period: 2018-2019
Funding Institution: Madrid Regional Government
Dr. A. Orozco

Programme: Talent Attraction Programme – Modality 2
Period: 2018-2019
Funding Institution: Madrid Regional Government
Dr. I. Papadimitriou

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

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

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

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

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

3. Scientific results

3.1. Publications

1. N. Boaretto, J. Almenara, A. Mikhalchan, R. Marcilla, J.J. Vilatela. *A Route to high-toughness battery electrodes.* **ACS Applied Energy Materials 2**, 5889-5899, 2019.
2. Z. Zhang, X. Li, Y. Yuan, Y.T. Pan, D.Y. Wang, R. Yang. *Confined dispersion of Zinc Hydroxystannate nanoparticles into layered Bimetallic Hydroxide nanocapsules and its application in flame-retardant epoxy nanocomposites.* **ACS Applied Materials and Interfaces 11**, 40951-40960, 2019.
3. X.L. Qi, D.D. Zhou, J. Zhang, S. Hu, M. Haranczyk, D.Y. Wang. *Simultaneous improvement of mechanical and fire-safety properties of polymer composites with phosphonate-loaded MOF additives.* **ACS Applied Materials and Interfaces 11**, 20325-20332, 2019.
4. L. Zhang, S. Chen, Y.T. Pan, S. Zhang, S. Nie, P. Wei, X. Zhang, R. Wang, D.Y. Wang. *Nickel metal–organic framework derived hierarchically mesoporous nickel phosphate toward smoke suppression and mechanical enhancement of Intumescent flame retardant wood fiber/poly (lactic acid) composites.* **ACS Sustainable Chemistry and Egineering 7**, 9272-9280, 2019.
5. H. Liu, I. Papadimitriou, F.X. Lin, J. LLorca. *Precipitation during high temperature aging of Al–Cu alloys: A multiscale analysis based on first principles calculation.* **Acta Materialia 167**, 121-135, 2019.
6. C. Cepeda, M. Castillo, M.T. Pérez-Prado. *Origin of the low precipitation hardening in magnesium alloys.* **Acta Materialia 165**, 164-176, 2019.
7. D. Shi, M.T. Pérez-Prado, C. Cepeda. *Effect of solutes on strength and ductility of magnesium alloys.* **Acta Materialia 180**, 218-230, 2019.
8. J.Y. Wang, N. Li, R. Alizadeh, M.A. Monclús, Y.W. Cui, J.M. Molina, J. LLorca. *Effect of solute content and temperature on the deformation mechanisms and critical resolved shear stress in Mg-Al and Mg-Zn alloys.* **Acta Materialia 170**, 155-165, 2019.
9. G. Esteban, E. Martínez, J. Segurado, L. Capolungo, J. LLorca. *An atomistic investigation of the interaction of dislocations with guinier-preston zones in Al-Cu alloys.* **Acta Materialia 162**, 189-201, 2019.
10. M. Iragi, C. Pascual, A. Esnaola, C.S. Lopes, L. Aretxabaleta. *Ply and interlaminar behaviours of 3D printed continuous carbon fibre-reinforced thermoplastic laminates; effects of processing conditions and microstructure.* **Additive Manufacturing 30**, 100884, 2019.
11. N.U. Rahman, L. Capuano, S. Cabeza, M. Feinaeugle, A. Garcia-Junceda, M.B. de Rooij, D.T. Matthews, G. Walmag, I. Gibson, G.R. Romer. *Directed energy deposition and characterization of high-carbon high speed steels.* **Additive Manufacturing 30**, 100838, 2019.
12. A. Martin, C. Cepeda, M.T. Pérez-Prado. *Gas atomization of gamma TiAl alloypowder for additive manufacturing.* **Advance Engineering Materials 22**, 1900594, 2019.

13. V. Fernandez, D. Sánchez, J.P. Fernández, A.L. Cortajarena, P.B. Coto, R.D. Costa. *Deciphering limitations to meet highly stable bio-hybrid light-emitting diodes.* **Advance Functional Materials 29,** 1904356, 2019.
14. E. Fresta, J.M. Carbonell, J.Y. Yu, D. Armentano, J. Cano, M. Viciano-Chumillas, R.D. Costa. *Deciphering the electroluminescence behavior of Silver(I)-complexes in light-emitting electrochemical cells: Limitations and solutions toward highly stable devices.* **Advance Functional Materials 29**, 1901797, 2019.
15. E. Fresta, M.D. Weber, J. Fernandez, R.D. Costa. *White light-emitting electrochemical cells based on deep-red Cu(I) complexes.* **Advance Optical Materials 7**, 1900830, 2019.
16. E. Fresta, J. Fernández, B. Gil, P. Montaño, J.R. Berenguer, M.T. Moreno, P.B. Coto, E. Lalinde, R.D. Costa. *Versatile homoleptic naphthyl-acetylide heteronuclear [Pt2M4 (C- C-Np) 8] (M= Ag, Cu) phosphors for highly efficient white and nir hybrid light-emitting diodes.* **Advance Optical Materials 8,** 1901126, 2019.
17. E. Menga, M.J. Sánchez, I. Romero, S. Hernández. *A sample-based approach to estimate the dynamic loads of components with nonlinear uncertain interfaces.* **Aerospace Science and Technology 87**, 369-378, 2019.
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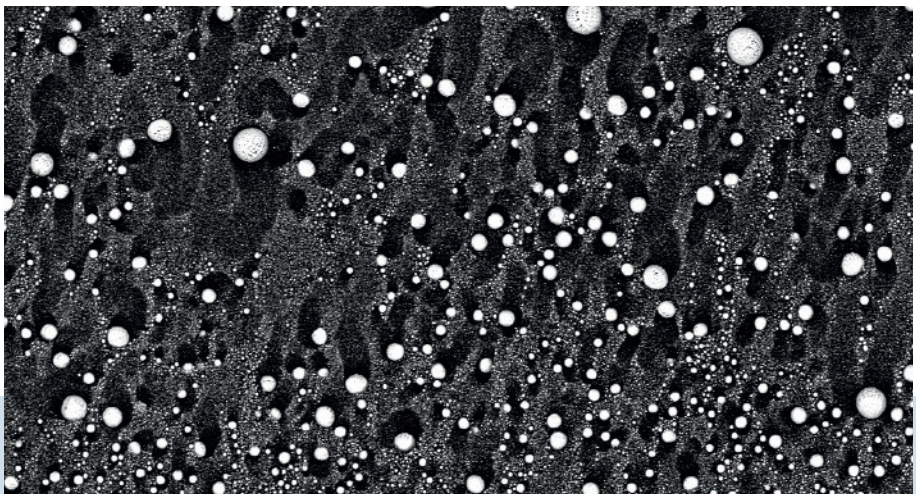

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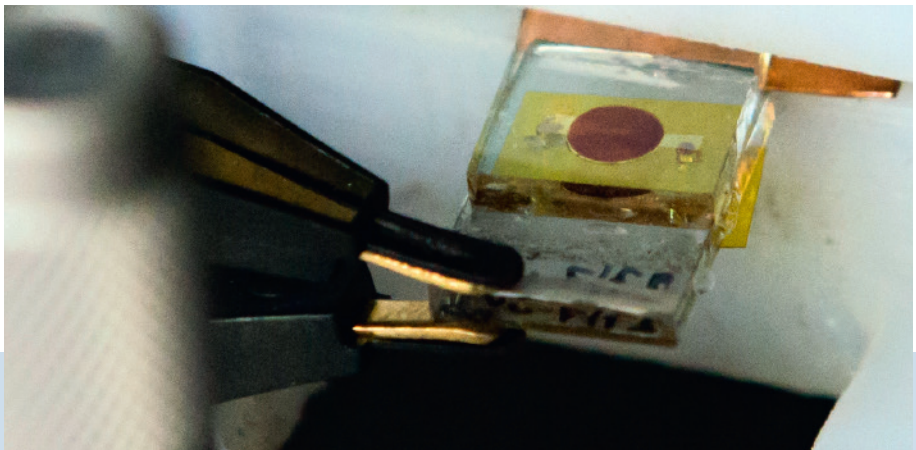

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3.2. Book chapters

1. R. Paul, M. Vincent, V. Etacheri, A.K. Roy. *Carbon nanotubes, Graphene, porous Carbon and hybrid Carbon materials: Synthesis, properties and functionalization for efficient energy storage.* In **Carbon Based Nanomaterials for Advanced Thermal and Electrochemical Energy Storage and Conversion. Science Direct**, 1-24, 2019.
2. A. Monreal-Bernal, M. Bidikoudi, R.D. Costa. *Carbon nanotubes in hybrid photovoltaics: dye sensitized and perovskites solar cells*. In **Carbon based nanomaterials for advanced thermal and electrochemical energy storage and conversion. Science Direct**, 201-248, 2019.
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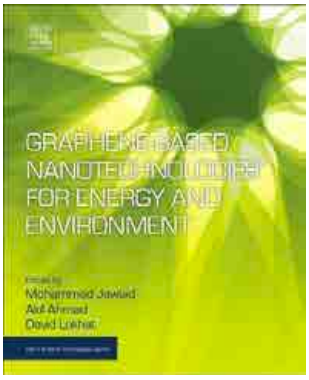
5. R.N. Gayen, V.S. Avvaru, V. Etacheri*. Carbon based integrated devices for efficient photo-energy conversion and storage.* In **Carbon Based Nanomaterials for Advanced Thermal and Electrochemical Energy Storage and Conversion**. **Science Direct**, 357-374, 2019.
6. A. Cruzado, J. LLorca, J. Segurado. *Computational micromechanics modelling of polycrystalline superalloys: application to Inconel*. In **Integrated computational materials engineering (ICME) - Advancing Computational and Experimental Methods**. **Springer Nature Switzerland AG**, 718, 2019.



3.3. Patent applications

1. *Nanowires network*. IMDEA Materials Institute. Patent application number EP19382996.7 (13 November 2019)
2. *Long-living bio Light-Emitting Diode*. IMDEA Materials Institute. Patent application number EP19382428.1 (29 May 2019)
3. *Sulfur cathodes protected with hybrid solid-electrolyte interfaces for high performance Li-S batteries.* IMDEA Materials Institute. Patent application number EP19382688.0 (6 August 2019)

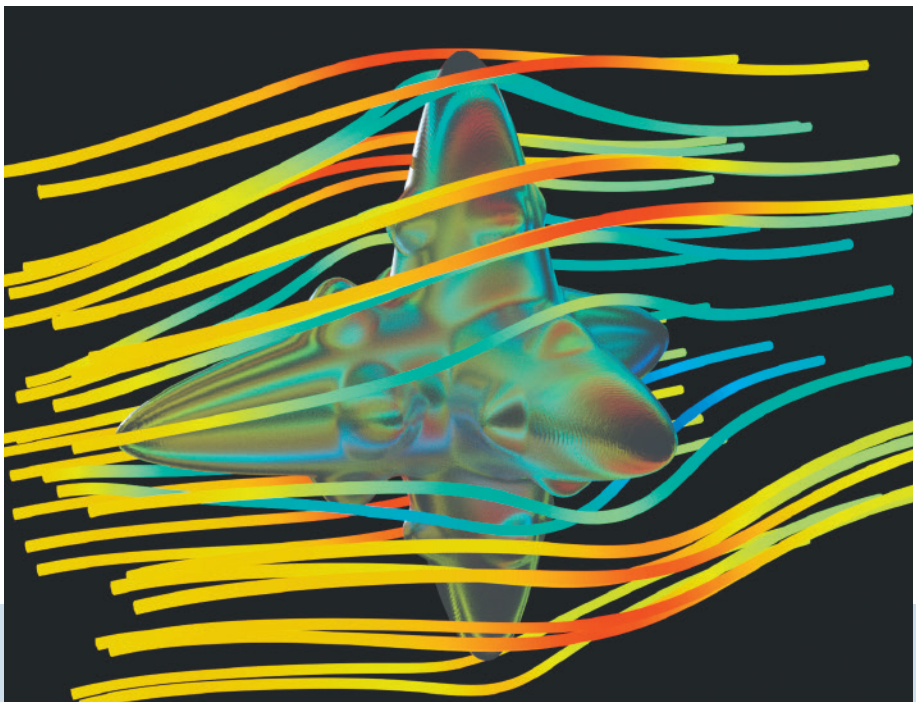
3.4. Software registered

1. *IRIS*. IMDEA Materials Institute and Technical University of Madrid. Registro Territorial de la Propiedad Intelectual, Comunidad de Madrid (23 May 2019).

3.5. International Conferences

Invited and plenary talks

1. *"Metal-ceramics nanolaminates: A new paradigm in metal-ceramic composites"*, J. LLorca, **XV Scientific Workshop of the Alicante Materials Institute**, Alicante, Spain, January 2019.
2. *"Mg research at IMDEA Materials started (as if) by MagIC"*, T. Pérez-Prado, **Scientific Colloquium in Honor of Prof. K. Kainer**, Hamburgo, Germany, January 2019.
3. *"Multiscale modelling of precipitation in metallic alloys"*, H. Liu, I. Papadimitriou, F.X. Lin, J. LLorca, **18th Gesellschaft für Angewandte Mathematik und Mechanik Seminar on Microstructures**, Berlin, Germany, January 2019.



4. *"Nanoscale engineering of materials and interfaces for high performance rechargeable batteries*", V. Etacheri, **Meeting on Nanochemistry and Nanotechnology (NANOUCO)**, Córdoba, Spain, January 2019.
5. *"Bottom-up multiscale modelling strategies to discover new materials"*, J. LLorca, **International Workshop "Energy and Nanomaterials"**, Tokyo, Japan, February 2019.
6. *"White lighting with hybrid materials",* R. Costa*,* **International Workshop "Energy and Nanomaterials"**, Tokyo, Japan, February 2019.
7. *"Energy-entropy-momentum integrators for nonlinear solid and fluid mechanics"*, I. Romero, **1st SFB International Workshop "Taming Complexity in Partial Differential Systems"**, Viena, Austria, February 2019.
8. *"Thermodynamically consistent integrators for nonlinear solid and fluid mechanics"*, I. Romero, **Congreso Bienal de la Real Sociedad Matemática Española**, Santander, Spain, February 2019.
9. *"Development of Al alloys for additive manufacturing",* S. Milenkovic, **Conference on 3D printing**, Rome, Italy, March 2019.
10. *"Fracture behavior of metal-ceramic and metal-metal nanolaminates ",* J. Molina, **TMS 2019, 148th Annual Meeting and Exhibition**, Texas, USA, March 2019.
11. *"High-throughput investigation of strength and creep in Mg alloys through micromechanical testing "*, **TMS 2019, 148th Annual Meeting and Exhibition**, Texas, J. Molina, N. Li, San Antonio, USA, March 2019.
12. *"Slip transfer at grain boundaries in pure Al"*, R. Alizadeh, T. Bieler, J. Molina, J. LLorca, **TMS 2019, 148th Annual Meeting and Exhibition**, Texas, USA, March 2019.
13. *"Innovative reactive infiltration method for production of fine grained iron aluminides",* S. Milenkovic, **Metallurgical & Materials Engineering Congress of South-East Europe (MME SEE 2019)**, Belgrade, Serbia, March 2019.
14. *"CNT fibres as macromolecular networks"*, J.J. Vilatela, **Workshop on Single Wall Carbon Nanotubes & related materials**, Texas, USA, April 2019.
15. *"A multiscale modelling strategy to predict precipitate stability, nucleation and growth in metallic alloys"*, H. Liu, I. Papadimitriou, B. Bellón, F.X. Lin, J. LLorca, **MRS Spring Meeting**, Phoenix, USA, April 2019.
16. *"Application of machine learning tools for quantitative 3D & 4D in material science!",* F. Sket, **Schloss Dagsthul Seminar on Computer Vision and Analysis**, Wadern, Germany, April 2019.
17. *"CNT fibres: materials science challenges and perspectives for industrial implementation",* J.J. Vilatela*,* **International Workshop on Graphene and Carbon Nanotubes in Experimental Mechanics**, Manchester, United Kingdom, May 2019.
18. *"Hybrid lighting and photovoltaic devices"*, R.D. Costa, **Liebig Meeting**, Frankfurt, Germany, May 2019.
19. *"Designing microstructures by additive manufacturing: the intrinsic heat treatment"*, T. Pérez-Prado, **TRATERMAT 2019**, Castellón, Spain, June 2019.
20. *"Impresión 3D de metales"*, T. Pérez-Prado, **Encuentro Ciencia y Sector Empresarial**, Madrid, Spain, June 2019.
21. *"Nano-hybrid as nano flame retardant to polymers: Opportunities and challenges",* D.Y. Wang, **FRPM19 Conference**, Turku, Finland, June 2019.

22. *"Physical simulation of friction stir processing"*, I. Sabirov, **XI Annual Scientific Workshop of UNIPRESS**, Warsaw, Poland, June 2019.
23. *"Almacenamiento, captación y transferencia de energía en materiales compuestos"*, J.J. Vilatela, **MATCOMP 2019**, Vigo, Spain, July 2019.
24. *"Carbon nanotube fibres for electrical cable usage",* M. Vila*,* **UltraWire Workshop 2019**, Cambridge, United Kingdom, July 2019.
25. *"Magnesium alloys",* T. Pérez-Prado*,* **Materials Processing Workshop**, Vigo, Spain, July 2019.
26. *"Multifunctionally fire-retardant polymer composites: From molecular design to high performance",* D.Y. Wang*,* **ACEX2019 Conference***,* Athens, Greece, July 2019.
27. *"Using general material constitutive relations in numerical methods for structural models: algorithms and variational basis"*, I. Romero, **International Conference Challenges on Mathematical Architecture Theory, Modeling and Applications**, Madrid, Spain, July 2019.
28. *"First principles calculation of the Al-rich part of Al-Cu phase diagram",* S. Liu, I. Papadimitriou, J. LLorca, **PRISMS Annual Meeting,** Dearborn, USA, August 2019.
29. *"Next generation rechargeable batteries based on defect and interface engineered electrode*", V. Etacheri, **ICAM Conference 2019**, Kottayam, India, August 2019.
30. *"CNT fibre development at IMDEA"*, J.J. Vilatela, **Cambridge Aerogel Process**, Cambridge, United Kingdom, September 2019.
31. *"Macroscopic fibres of CNTs: molecular control, hierarchical structure and applications in energy storage",* M. Vila, **Conference NANOMAT 2019**, Prague, Czech Republic, September 2019.
32. *"A continuum model for the prediction of diffusional creep in metallic polycrystalline aggregates at high temperatures and low stresses",* J. Segurado, **COMPLAS 2019**, Barcelona, Spain, September 2019.
33. *"Discovery of nanoporous materials for energy applications"*, M. Haranczyk, **2nd RSC-BMCS/RSC-CICAG Artificial Intelligence in Chemistry,** Cambridge, United Kingdom, September 2019.
34. *"Hybrid lighting and photovoltaic devices",* R. Costa*,* **EUROMAT 2019**, Stockholm, Sweden, September 2019.
35. *"On the formation of grain boundaries during polycrystalline solidification"*, D. Tourret, **EUROMAT 2019**, Stockholm, Sweden, September 2019.
36. *"Multiscale modelling of precipitation hardening in Al-Cu alloys: dislocation dynamics simulations and experimental validation"*, R. Santos, B. Bellón, G. Esteban-Manzanares, J. Segurado, J. LLorca, **XV International Conference on Computational Plasticity (COMPLAS 2019),** Barcelona , Spain , September 2019.
37. *"On the effect of grain boundaries on the strength of polycrystals: Hall-petch revisited",* S. Haouala, S. Lucarini, J. Segurado, J. LLorca, **XV International Conference on Computational Plasticity (COMPLAS 2019),** Barcelona, Spain, September 2019.
38. *"Precipitate strengthening in Mg alloys: Atomistic simulations and experimental observations"*, G. Esteban-Manzanares, I. Papadimitriou, R. Alizade, A. Ma, J.

LLorca, **XV International Conference on Computational Plasticity (COMPLAS 2019)**, Barcelona, Spain, September 2019.

39. *"Multiscale modelling of precipitation hardening in metallic alloys"*, J. LLorca, **Dislocations 2019**, Haifa, Israel, September 2019.
40. *"Superior hybrid light-emitting diodes and solar cells using organometallo-metal oxide nanoparticles",* R. Costa*,* **2019 CCMR Conference**, Gyeonggi-do, Korea South, September 2019.
41. *"A roadmap for multiscale modelling of precipitation and precipitation hardening in metallic alloys from first principles simulations"*, J. LLorca, **Computational Modelling of Complex Materials Across the Scales 2019**, Glasgow, United Kingdom, October 2019.
42. *"Determination of precipitate strengthening in Al-Cu alloys through micropillar compression: Experiments and multiscale simulations"*, B. Bellón, R. Santos, S. Haouala, J. LLorca, **Nanomechanical Testing in Materials Research and Development VII,** Málaga, Spain, October 2019.
43. *"Interface: An attractive topic of flame retardant polymer (nano) composites"*, D.Y. Wang, **AOFSM3**, Shanghai, China, October 2019.
44. *"Multiscale modelling of precipitation and precipitation hardening in Al-Cu alloys from first principles simulations"*, J. LLorca, **2019 International Workshop on Materials Genomics**, Shanghai, China, October 2019.
45. *"On the use of multiscale modelling strategies to design precipitation-hardened Al alloys",* J. LLorca*,* **International Conference on Lightweight Materials and Manufacture,** Changsha Hunan, China, October 2019.
46. *"Precipitation hardening in light alloys: why is it more efficient in Al alloys than in Mg alloys?"*, J. LLorca, **9th International Light Metals Technology Conference,** Shanghai, China, October 2019.
47. *"2D materials for advanced applications",* E. Naderikalali*,* **ICFM & MFMS & INM 2019**, Chongqing, China, November 2019.
48. *"Multiscale modelling of composites: Towards virtual testing"*, C. González, **ICFM & MFMS & INM 2019**, Chongqin, China, November 2019.
49. *"Accelerating discovery of porous materials with data-driven approaches"*, M. Haranczyk, **10th China International Conference on Functional Materials and Applications**, Chongqing, China, November 2019.
50. *"Light-emitting electrochemical cells: Advances and challenges"*, R. Costa, **XVI Simposio de Investigadores Jóvenes RSEQ-Sigma Aldrich (Merck) 2019**, Valencia, Spain, November 2019.
51. *"Microplasticity of magnesium alloys",* T. Pérez-Prado*,* **LIGHTMAT 2019**, Manchester, United Kingdom, November 2019.
52. *"Multiscale modeling and integrated computational materials engineering at IMDEA Materials"*, D. Tourret, J. Segurado, **ICME Workshop organized by Airbus**, Toulouse, France, November 2019.
53. *"A coupled model of diffusional creep of polycrystalline solids based on climb of dislocations at grain boundaries",* J. Segurado*,* **MRS Winters Meeting**, Boston, USA, December 2019.

Regular contributions

1. *"Microstructure and mechanical characterization of thin bioactive PEO coatings fabricated on UFG CP Ti"*, H. Mora, I. Sabirov, M.A. Monclus, E. Matykina, R. Arrabal, J. Molina, **Nanobrucken 2019: A Nanomechanical Testing Conference**, Berlin, Germany, February 2019.
2. *"Using XPM for correlating Nb segregation with mechanical properties of cast Inconel 718",* A. Orozco, C. Gutiérrez, J. Molina*,* **Nanobruecken 2019-Nanomechanical testing conference**, Berlín, Germany, February 2019.
3. *"Discovery of new porous molecular materials through characterization of their building blocks"*, I. Gómez, **6th International Conference on Multifunctional, Hybrid and Nanomaterials**, Sitges, Spain, March 2019.
4. *"Enhanced interlaminar fracture toughness of woven carbon fabric/epoxy composites by interleaving fluffy CNT veils",* Y.F. Ou, **MATCOMP 2019**, Vigo, Spain, March 2019.
5. *"An analysis of the deformation and fracture mechanisms of Cu/Nb nanolaminates by in situ TEM mechanical tests",* Z. Liu, M.A. Monclús, L.W. Yang, M. Castillo, J. Molina, J. LLorca, **MRS Spring Meeting,** Phoenix, USA, April 2019.
6. *"Effect of nucleating particles on the microstructure of 7075 Al alloy manufactured by selective laser melting",* C. Galera, M. Montero, K. Vanmeensel, M. Godino, M.T. Pérez-Prado, J. LLorca, **MRS Spring Meeting,** Phoenix, USA, April 2019.
7. *"Simulation of Scatter and specimen size efect in fatigue life of metelas using computational micromechanics",* J. Segurado*,* **36 Encuentro del Grupo Español de Fractura**, Sevilla, Spain, April 2019.
8. *"High strain rate micromechanical testing of composite materials"*, M. Rueda, B. Beake, J. Molina. **COMPTEST 2019,** Lulea, Sweden, May 2019.
9. *"Developing powders by gas atomisation for laser-based additive manufacturing of Ti and Fe rich ultrafine eutectic alloys"*, A. Kumar, **CEIMP 2019**, Madrid, Spain, June 2019.
10. *"Developing powders for additive manufacturing of Ti and Fe rich ultrafine eutectic alloys"*, A. Kumar, **CEIMP 2019**, Madrid, Spain, June 2019.
11. *"High-throughput measurements for the micro-mechanical plastic deformation in Mg-Al alloy",* J.Y. Yang, J. LLorca, Y.W. Cui, **CALPHAD XLVIII**, Singapore, Singapore, June 2019.
12. *"MOFs derived hierarchical materials as multifunctional fire retardants for epoxy composites"*, J. Zhang, **FRPM19 Conference**, Turku, Finland, June 2019.
13. *"Small scale atomization of hastelloy X powder and its SLM procesability",* S. Milenkovic, **Jornadas ITP Aero - Conocimiento Tecnológico**, Bilbao, Spain, June 2019.
14. *"Multiscale modeling of dendritic growth using the dendritic needle network approach: Recent developments and future directions",* D. Tourret, **International Conference on Advances in Solidification Processes, ICASP-5,** Salzburg, Austria, June 2019.
15. *"Synthesis of new powders optimised for AM by atomization",* S. Milenkovic, A. Martin, C. Cepeda, M.T. Pérez-Prado, J. Molina, D. Tourret, M.L. Montero, K. Vanmeensel, **Jornadas ITP Aero - Conocimiento Tecnológico,** Bilbao, Spain, June 2019.

16. *"Aligned CNT fibres and multifilament fabrics: mechanical analysis and integration into structural composites"*, A. Mikhalchan, **Carbon 2019 Conference**, Lexington, USA, July 2019.
17. *"Carbon nanotube fibres: A micromechanical model and the challenges for their use in structural composites"*, J.J. Vilatela, **CNPComp Conference**, London, United Kingdom, July 2019.
18. *"Operando characterization of CNT fibre fabric-based electrodes and their application for high-toughness batteries"*, J.J. Vilatela, **NT19 Conference**, Wurzburg, Germany, July 2019.
19. *"Calibration of material models applied to impact mechanics using a new statistical approach"*, J.L. de Pablos, **Congress on Numerical Methods in Engineering (CMN 2019)**, Guimaraes, Portugal, July 2019.
20. *"Optimized computational methods for the calculation of dispersion diagrams"*, S. Sánchez, **Congress on Numerical Methods in Engineering (CMN 2019**), Guimaraes, Portugal, July 2019.
21. *"Comparison of Zn- and Mg-based scaffold structures for orthopedic applications"*, A. Kopp, I. Schestakow, M. Müther, T. Derra, M. Hinz, M. Li, J. Molina, J. LLorca, P. Schückler, L. Jauer, J. Schleifenbaum, P. Wen, N. Kröger, R. Smeets, L. Kluwe, P. Hartjen, M. Voshage, **11th Symposium on Biodegradable Metals,** Alicante, Spain, July 2019.
22. *"Estudio de la generación y evolución de daño en laminados de fibra de carbono sujetos a ciclado térmico y agentes corrosivos"*, I. Lizarralde, **MATCOMP 2019**, Vigo, Spain, July 2019.
23. *"Estudio de velocidad de resina y poros en procesos de moldeo por ruta líquida mediante tomografía rápida de rayos X",* J. Castro, **MATCOMP 2019**, Vigo, Spain, July 2019.

24. *"Fabricación de compuestos de fibra larga reciclada de carbono mediante inyección",* A. Fernández, M. Santangelo, J. Molina, C.S. Lopes, **MATCOMP 2019**, Vigo, Spain, July 2019.
25. *"High rate translaminar fracture toughness characterization in carbon fiber reinforced composite"*, C. González, **MATCOMP 2019**, Vigo, Spain, July 2019.
26. *"Interlaminar fracture toughness of 3D printed continuous-fibre reinforced polyamide"*, M. Iragi, C. Pascual, A. Esnaola, J. Aurrekoetxea, C.S. Lopes, **MATCOMP 2019**, Vigo, Spain, July 2019.
27. *"Longitudinal tensile failure mechanism in unidirectional FRP composites by means of computational micromechanics"*, M. Barzegar, C.S. Lopes, J. Costa, **MATCOMP 2019,** Vigo, Spain, July 2019.
28. *"Postprocessing-microstructure-calorimetry effects on the mechanical response of additive manufactured continuous-fibre reinforced polymers",* C. Pascual, M. Iragi, A. Fernández, L. Aretxabaleta, C.S Lopes, **MATCOMP 2019**, Vigo, Spain, July 2019.
29. *"Integration schemes that preserve the two laws of thermodynamics"*, D. Portillo, I. Romero, **International Congress on Industrial and Applied Mathematics**, Valencia, Spain, July 2019.
30. *"Phase-field modeling of melt pool solidification",* F. Yu, Y. Wei, D. Tourret, **4th International Symposium on Phase-Field Modelling in Materials Science,** Bochum, Germany, July 2019.
31. *"Multiscale simulation of precipitation in Al-Cu alloys",* H. Liu, I. Papadimitriou, B. Bellón, F.X. Lin, J. LLorca, **4th International Symposium on Phase-Field Modelling in Materials Science**, Bochum, Germany, July 2019.
32. *"Phase-field as a benchmark for other models of solidification and microstructure evolution",* D. Tourret, **International Symposium on Phase-Field Modelling in Materials Science**, Bochum, Germany, July 2019.
33. *"CNT fiber veil interleaved carbon fiber/expoxy laminate composite",* Y. Ou, **ICCM22**, Melbourne, Australia, August 2019.
34. *"Synthesis of continuous macroscopic fibres and doping in the point of synthesis",* M. Vila, **NANOTEC 19**, Zaragoza, Spain, August 2019.
35. *"Alignment and reinforcing potential of multifilament CNT fabrics",* A. Mikhalchan, **ICCM-22 International Conference**, Melbourne, Australia, August 2019.
36. *"Effect of nucleating particles on the microstructure of 7075 Al alloy manufactured by selective laser melting"*, C. Galera, M. Montero, K. Vanmeensel, M. Godino, M.T. Perez-Prado, J. LLorca, **Alloys for Additive Manufacturing Symposium 2019,** Stockholm, Sweden, September 2019.
37. *"A numerical framework to analyze fracture in composite materials: from simulated crack resistance curves to homogenized softening laws",* M. Herráez, C. González, C.S. Lopes, **7th Thematic Conference on the Mechanical Response of Composites (ECCOMAS Composites 2019)**, Girona, Spain, September 2019.

38. *"Longitudinal tensile failure mechanism in unidirectional FRP composites by means of computational micromechanics"*, M. Barzegar, C.S. Lopes, J. Costa, **7th Thematic Conference on the Mechanical Response of Composites (ECCOMAS Composites 2019)**, Girona, Spain, September 2019.
39. *"Micromechanical modeling of composite ply incorporating a strain rate dependent constitutive model informed by a novel micromechanical testing technique"*, M. Rueda, B. Beake, C. González, J. Molina, **7th Thematic Conference on the Mechanical Response of Composites (ECCOMAS Composites 2019)**, Girona, Spain, September 2019.
40. *"Modelling and experimental analysis of fatigue of Mg-RE alloys"*, M. Zhang, H. Zhang, A. Ma, J. LLorca, **EUROMAT 2019,** Stockholm , Sweden, September 2019.
41. *"Rainbow light-emitting electrochemical cells based on Cu(I) complexes"*, E. Fresta, **EUROMAT 2019**, Stockholm, Sweden, September 2019.
42. *"Ultrafine eutectic Ti-based alloys for additive manufacturing"*, J. Gussone, **Workshop on Coherence at ESRF-EBS**, Grenoble, France, September 2019.
43. *"Understanding lithium storage mechanism in nanostructured MnO2@CNT hybrid by in-situ synchrotron X-ray scattering study",* M. Rana*,* **ESRF -EBS Workshop 2019**, Grenoble, France, September 2019.
44. *"Understanding lithium storage mechanism in nanostructured MnO2@CNT hybrid by in-situ synchrotron X-ray scattering study",* M. Rana*,* **EMRS fall 2019**, Warsaw, Poland, September 2019.
45. *"A numerical study of specimen size effects in polycrystalline metals",* J. Segurado, **Jornadas ITP Aero - Conocimiento Tecnológico**, Mondragón, Spain, September 2019.
46. *"Evolution of microstructure and mechanical properties during conventional and ultra-fast heating of a low carbon steel: the effect of soaking time",* M.A. Valdés, F. Vercruysse, M. Monclus, J. Molina, R. Petrov, I. Sabirov, **Materials Science and Technology 2019 Conference**, Portland, USA, September-October 2019.
47. *"Effect of lamellar orientation and width on the strength and operating deformation mechanisms of fully lamellar TiAl alloys determined by micropillar compression",* C. Gutiérrez, I. Sabirov, T. Pérez-Prado, J. Molina*,* **Nanomechanical Testing in Materials Research and Development VII,** Torremolinos, Spain, October 2019.
48. *"Microstructure and high temperature mechanical properties of hard tasin coatings"*, M. Monclús, L. Yang, I. López, R. González, E. Meletis, J. LLorca, J. Molina, **Nanomechanical Testing in Materials Research and Development VII**, Torremolinos, Spain, October 2019.
49. *"New instrumentation and analysis methodology for nano-impact testing",* M. Rueda, B. Beake, J. Molina, **Nanomechanical Testing in Materials Research and Development VII**, Torremolinos, Spain, October 2019.
50. *"MoS_2@CNT hybrid for free-standing charge storage: Mechanistic investigations on growth and charge storage mechanism",* M. Rana, **CESEP 2019 Conference**, Alicante, Spain, October 2019.

51. *"Understanding microstructural phenomena in carbon nanotube fibres and their hybrids using in-situ synchrotron X-ray scattering techniques",* M. Rana, **IX AUSE Conference**, Barcelona, Spain, October 2019.
52. *"A realistic route to intrinsic fire safety of Li-ion batteries and highlights of electrolyte oxygen consumption calorimetry",* A. Yusuf*,* **ICFM & MFMS & INM 2019**, Chongqing, China, November 2019.
53. *"Bioinspired iron-loaded polydopamine nanospheres as green flame retardant for epoxy resin via free radical scavenging and catalytic charring",* L. Zhang, **ICFM & MFMS & INM 2019,** Chongqing, China, November 2019.
54. *"Functionalized LDH in Epoxy Resins"*, J. de la Vega, **ICFM & MFMS & INM 2019**, Chongqing, China, November 2019.
55. "Forgotten materials and promised materials in additive manufacturing", M.A. Rodiel, **2nd Congress of Additive Manufacturing (ADITIVA 4.0)**, Murcia, Spain, December 2019.
56. *"Effects of dynamic failure and local peak stress in UD composites",* M. Barzegar, J. Costa, C.S. Lopes, **FiBreMoD School and Conference**, Leuven, Belgium, December 2019.
57. *"High strain rate micromechanical testing of composite materials"*, M. Rueda, B. Beake, J. Molina, **Micro Materials User Meeting 2019**, Southampton, United Kingdom, December 2019.

Membership in organising committees

1. **International Workshop Energy and Nanomaterials**, R. Costa (Co-Organiser). Tokyo, Japan, February 2019, February 2019.
2. **Annual TMS Meeting**. D. Tourret (Symposium Organiser). San Antonio, Texas, USA, March 2019.
3. **Materials for Health and Food Start-ups Brokerage event**, E. Troche and M.A. Rodiel (Co-Organisers), Madrid, Spain, June 2019.
4. **Workshop on Materials for Nuclear Applications. CEIDEN – MATERPLAT Technological Platforms**, E. Troche and M.A. Rodiel (Co-Organisers), Madrid, Spain, July 2019.
5. **International Congress of Thermal and surface treatments (TRATERMAT 2019)**. T. Perez-Prado (Member of the Scientific Committee). Castellón, Spain, July 2019.
6. **EUROMAT 2019**, S. Milenkovic and C. Capdevilla (Symposium Organiser). Stockholm, Sweden, September 2019.
7. **Women in 3D printing**, T. Perez-Prado (Co-Organiser), Madrid, Spain, October 2019.
8. **6th International Conference on Multi-Functional Materials and Structures (MFMS 2019)**. D.Y. Wang (Co-Chairman). Chongqing, China, November 2019.
9. **Functional Materials and Advanced Application Workshop & 1st Annual Meeting of Spain-China Joint Research Center of Advanced Materials**, D.Y. Wang (Chairman), Madrid, Spain, November 2019.
10. **MRS Fall Meeting**. D. Tourret (Symposium Organiser). Boston, USA, December 2019

3.6. Invited seminars and lectures

1. *"MOMTalks"*, R.D. Costa, **Materials Science Institute of Sevilla - CSIC**, Sevilla, Spain, January 2019.
2. *"Advances in hybrid optoelectronics for solar energy conversion* ", R.D. Costa, **INTA**, Torrejón de Ardoz, Spain, January 2019.
3. *"Macroscopic fibres of CNTs: Molecular control, hierarchical structure and applications in energy storage and composites*", J.J. Vilatela, **Waseda University**, Tokyo, Japan, February 2019.
4. *"Macroscopic fibres of CNTs: Molecular control, hierarchical structure and applications in energy storage and composites*", J.J. Vilatela, **National Institute of Advanced Industrial Science (AIST),** Tzukuba, Japan, February 2019.
5. *"Macroscopic fibres of CNTs: Molecular control, hierarchical structure and applications in energy storage and composites*", J.J. Vilatela, **Korea Institute of Science and Technology (KIST)**, Jeonbuk, South Korea, February 2019.
6. *"Multiscale modeling of strengthening mechanisms in metallic polycrystals: Effect of precipitates and gran boundaries"*, J. LLorca, **Ecole Polytechnique**, Palaiseau, France, February 2019.
7. *"New advances in physical simulation of metallurgical processes*", I. Sabirov, **University of Wollongong**, Wollongong, Australia, March 2019.
8. *"Invited lecture: Metal additive manufacturing technology*", S. Milenkovic, **Faculty of Technology and Metallurgy**, Belgrade, Serbia, March 2019.
9. *"Multiscale modelling of fiber-reinforced composites: Towards a bottom-up design approach"*, J. LLorca, **Institut für Textiltechnik RWTH**, Aachen, Germany, March 2019.
10. *"Multiscale characterization and modelling of Mg alloys for structural applications",* J. LLorca, J. Molina, **Meotec GmbH**, Aachen, Germany, March 2019.
11. *"FaXtor: A new fast tomography beamline for ALBA synchrotron–pre-design workshop, the material science perspective in 5 years*", F. Sket, **ALBA Synchrotron**, Cerdanyola del Valles, Spain, April 2019.
12. *"Recent advances in thin film lightning" at Material Science Seminar*", R. Costa, **University of La Rioja**, La Rioja, Spain, April 2019.
13. *"A roadmap for multiscale modelling of precipitation and precipitation hardening: Application to Al-Cu",* J. LLorca, **Department of Metallurgical and Materials Engineering School of Mines**, Colorado, USA, April 2019.
14. *"Models and numerical methods for solids with reinforcing fibers*", I. Romero, **2nd Technical University of Madrid (UPM) - Northwestern Polytechnical University (NPU) Workshop on Advanced Materials**, Madrid, Spain, May 2019.
15. *"White hybrid light-emitting diodes*", R. Costa, **University of Oviedo**, Oviedo, Spain, May 2019.
16. *"A roadmap for multiscale modelling of precipitation and precipitation hardening: Application to Al-Cu",* J. LLorca, **Department of Materials Oxford University,** Oxford, United Kingdom, May 2019.

17. *"Virtual testing of metallic polycrystals",* J. LLorca, **Institute of Fundamental Technological Research Polish Academy of Sciences**, Warsaw, Poland, May 2019.
18. *"Links between beams and solids: New variational principles and their finite element discretization*", I. Romero, **Technical University of Madrid**, Madrid, Spain, June 2019.
19. "Metallic materials for additive manufacturing". M.A. Rodiel, **Madrid Automotive Cluster**, Madrid, Spain, June 2019.
20. *"Multiscale modeling of strengthening mechanisms in metallic polycrystals: effect of precipitates and gran boundaries",* J. LLorca, **Department of Engineering Science Université du Luxembourg,** Luxembourgh, June 2019.
21. *"Protein-polymer phosphors for energy-related applications"*, R.D. Costa, **University of Hannover**, Hannover, Germany, June-July 2019.
22. *"White hybrid light-emitting diodes*", R. Costa, **University of Oviedo**, Oviedo, Spain, June-July 2019.
23. *"Bio-Hybrid Light-emitting Diodes: Origins, Advances and Outlook* ", R. Costa, **Complutense University of Madrid**, Madrid, Spain, June-July 2019.
24. *"Design and use of hybrid materials for energy-related applications*", R. Costa, **Eberhard Karls University of Tübingen**, Stuttgart, Germany, July 2019.
25. *"Summer School On Computational Materials Science Across Scales",* J. Segurado, **Texas A&M University**, College Station, USA, July-August 2019.
26. *"Designing protein-polymer phosphors for energy-related applications"*, R.D. Costa, **Stockholm University**, Stockholm, Sweden, September 2019.
27. *"5th International Fall School on Organic Electronics IFSOE-2019*", R.D. Costa, **University of Moscu**, Moscu, Rusia, September 2019.
28. *"High-throughput experimental techniques to measure the CRSS for slip and twinning in Mg and Mg alloys",* J. LLorca, **Faculty of Mechanical Engineering**, Haifa, Israel, September 2019.
29. *"Solidification across length and time scales: From atoms to dendrites to grain microstructures*", D. Tourret, **Lorraine University - Institut Jean Lamour**, Nancy, France, October 2019.
30. *"CNT fibres as macromolecular networks*", J.J. Vilatela, **Aalto University**, Helsinki, Finland, October 2019.
31. *"Deconstructing magnesium plasticity*", T. Pérez-Prado, **Lovaine Catholic University**, Lovaina, Belgium, October 2019.
32. *"Progress of Nano-fire retardant*", D.Y. Wang, **Leibniz-Institut für Polymerforschung (IPF)**, Dresden, Germany, October 2019.
33. *"Multiscale modeling of strengthening mechanisms in metal polycrystals: effect of precipitates and gran boundaries",* J. LLorca, **Department of Engineering Mechanics**, Beijing, China, October 2019.
34. *"High-throughput experimental techniques to measure the CRSS for slip and twinning in Mg and Mg alloys",* J. LLorca, **Materials Genomics Institute**, Shanghai, China, October 2019.

35. *"Microstructure formation during the solidification of structural alloys*", D. Tourret, **Argonne National Laboratory - Center for Nanoscale Materials**, Lemont, USA, November 2019.
36. *"Advancing chemistry in Spain: Early Careers ERC Researchers*", R.D. Costa, **University of Islas Baleares,** Palma, Spain, November 2019.
37. *"X-ray tomography for the characterization of processing defects and damage due to mechanical testing in fibre reinforced composite materials",* F. Sket*,* **Webinar AEMAC 2019**, Getafe, Spain, October 2019.
38. *"High-throughput investigation of plastic anisotropy in Mg alloys*", J. Molina, **ETH**, Zurich, Switzerland, December 2019.
39. *"Mechanisms of precipitation hardening in Mg alloys: experimental evidence and atomistic simulations",* J. LLorca, **RWTH,** Aachen, Germany, December 2019.

3.7. Awards

1. JOM Best Paper Award, The Minerals, Metals and Materials Society (TMS), March 2019, **J. Molina, M. Monclús, J. LLorca.**
2. Real Spanish Society of Chemistry (RSEQ) Young Researcher Award, ChemPubSoc, March 2019, **R.D. Costa**.
3. Materials Research Society Fellow, Materials Research Society, April 2019, **J. LLorca.**
4. FEMS Materials Science & Technology 2019 Award, EUROMAT 2019, August 2019, **R.D. Costa.**
5. Youth National Award 2019 – Environment INJUVE, Ministry of Health, October 2019, **A. Fernández.**

3.8. Seminars

1. *"Microstructured magnetorheological elastomers and instabilities"* **Prof. Kostas Danas** (from The Ecole Polytechnique in Paris). January 2019.
2. "*On the radiation-induced origin of hardening and embrittlement in nuclear steels*" **Dr. Lorenzo Malerba** (from CIEMAT in Madrid). January 2019.
3. *"Microstructure control during laser additive manufacturing – what possibilities do we have?"* **Dr. Christian Leinenbach** (from EMPA - Swiss Federal Laboratories for Materials Science & Technology in Zurich). January 2019.
4. *"An example case for Machine-Learning in Materials Science: A neural networks based framework for 'smart' computational micromechanics of composites"* **Joshua Kiefer** (from Delft University of Technology in Holand). February 2019.
5. *"Protein-based acoustic and photon spectroscopy: Applications from biomaterials to protein design"* **Dr. Juan Pablo Fuenzalida** (from the University of Münster in Germany). February 2019.
6. *"Biomaterial physical properties in tissue regeneration"* **Dr. Amaia Cipitria** (from Max Planck Institute of Colloids and Interfaces in Potsdam in Germany). February 2019.
7. *"Thermoplasticity through the scales"* **Prof. Eric Charkaluk** (from CNRS – Laboratoire de Mécanique des Solides & from the Ecole Polytechnique in France). February 2019.
8. *"Atomistic description of grain boundary dislocations and related processes"* **Prof. Ana Serra** (from Polytechnic University of Catalonia in Spain). February 2019.
9. *"Stablishing predictive capability for progressive damage and failure in composite structures: A perspective on Virtual Testing"* **Andrew Cole Bergan** (from the NASA Langley Research Center). May 2019.
10. *"The influence of cooling rate on and 'chemical composition and mechanical properties in a Ni based superalloy"* **Dr. Muzi Li** (from IMDEA Materials Institute in Spain). May 2019.
11. *"Micromechanical response during biaxial load path changes of stainless steel: insitu neutron diffraction and multi-scale modeling"* **Dr. Manas Upadhyay** (from Ecole Polytechnique in Paris). June 2019.
12. *"In-situ x-ray imaging studies of solidification"* **Dr. Enzo Liotti** (from University of Oxford in UK). July 2019.
13. "Doped carbon nanostructures for electrochemical energy devices" **Dr. Ysmael Verde** (from TECNM in México). September 2019.
14. *"FFT-based polycrystal mechanics models combined with data analytics and experimental integration"* **Dr. Ricardo Lebensohn** (from Los Alamos National Laboratory in USA). September 2019.
15. *"Critical resolved shear stresses (CRSS) of Hexagonal Titanium from nanoindentation optimization"* **Zhouwen Zhao** (from Michigan State University in USA). July 2019.

16. *"Physics-based models for fatigue damage"* **Dr. Gustavo M. Castelluccio** (from Cranfield University in UK). October 2019.
17. *"Interfacial modification in nanocomposites to tailor Functionalities"* **Prof. Sabu Thomas** (from Mahatma Gandhi University in India). October 2019.
18. *"Outstanding radiation resistance of Tungsten-based High Entropy Alloys"* **Dr. Enrique Martínez** (from Los Alamos National Laboratory in USA) November 2019.
19. *"Meeting climate targets with both eyes open: How can we meet the growing demand for materials without destroying the environment?"* **Dr. Ana González** (from Cambridge University in UK). November 2019.
20. *"Homogenization methods for elasto-viscoplastic composites"* **Dr. Michalis Agoras** (from the University of Thessaly in Greece). December 2019.

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: Protein-Polymer materials for energy- and medical-related applications.
Description: Family of flexible and rigid polymer coatings, in which fluorescent proteins (FPs) and enzymes are easily introduced. The bio-functionality is preserved over years under ambient conditions and several months under device/reactor operation conditions.
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: 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: 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: 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: 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: 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

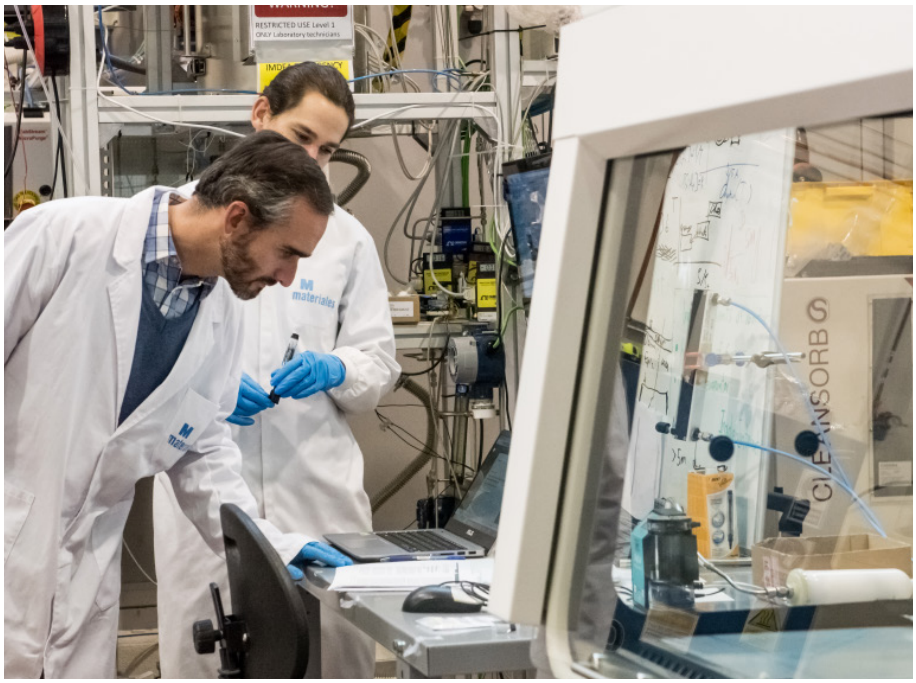
Title: MULTIFOAM.
Description: Simulation tool developed within the framework of computational micromechanics by IMDEA Materials to predict the mechanical behavior of low to medium density foams with open and closed-cell microstructure.
Opportunity: Software license

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



5. Training, communication and outreach

5.1. Theses

PhD Theses

1. *"Development and optimization of the properties of gamma/gamma Co-based superalloys for high temperature applications"*
   Student: Marta Cartón
   Carlos III University of Madrid
   Advisors: Prof. Jose M. Torralba and Prof. Mónica Campos
   Date of defense: January 2019

2. *"Microstructure-properties relations for hierarchically structured CNT fibres"*
   Student: Juan Carlos Fernández
   Technical University of Madrid
   Advisor: Dr. Juan Jose Vilatela
   Date of defense: January 2019

3. *"Fast mapping of microstructure and mechanical properties in Titanium alloys by kinetic diffusion multiple approach"*
   Student: ChuanYun Wang
   Technical University of Madrid
   Advisor: Dr. Teresa Pérez-Prado
   Date of defense: March 2019

4. *"Development of new Cr-based hardmetals by liquid phase sintering and spark plasma sintering"*
   Student: Xiangxing Deng
   Carlos III University of Madrid
   Advisors: Dr. Andrea García-Junceda
   Date of defense: March 2019

5. *"Effect of graphene nanoplatelets and carbon nanotubes in PEEK and PEEK/carbon fibre composites"*
   Student: Ángel Alvaredo
   Carlos III University of Madrid
   Advisors: Dr. Roberto Guzman and Dr. Juan Pedro Fernández
   Date of defense: June 2019

6. *"A study of the factors influencing air removal in Out-of-Autoclave processing of composites"*
   Student: Juan José Torres
   Technical University of Madrid
   Advisors: Prof. Carlos González and Dr. Federico Sket
   Date of defense: July 2019

7. *"Development and validation of numerical modelling approaches for triaxially-braided composites"*
   Student: Alejandro Garcia-Carpintero
   Technical University of Madrid
   Advisors: Porf. Carlos González and Dr. Claudio S. Lopes
   Date of defense: September 2019

8. *"High throughput investigation of diffusion and solid solution hardening of HCP Mg alloys"*
   Student: Jingya Wang
   Technical University of Madrid
   Advisor: Prof. Javier LLorca
   Date of defense: September 2019

9. *"Analytical and experimental study of the wettability of Si against different substrates"*
   Student: Almudena Casado
   Carlos III University of Madrid
   Advisors: Dr. Srdjan Milenkovic and Prof. José M. Torralba
   Date of defense: September 2019

10. *"Manufacturing of the ZAMAC 2 alloy by powder metallurgy and consolidation by extrusion and field assisted hot pressing"*
Student: Kamila Kazmierczak
Santa Catarina State University
Advisors: Dr. C.E. Costa and Dr. Srdjan Milenkovic
Date of defense: September 2019

11. *"Atomistic modeling of the strengthening mechanisms in FCC and HCP metals"*
Student: Gustavo Esteban
Technical University of Madrid
Advisor: Dr. Javier Segurado and Prof. Javier LLorca
Date of defense: November 2019

12. *"Crystal plasticity simulation of the thermo-mechanical behavior in polycrystalline metals"*
Student: Jifeng Li
Technical University of Madrid
Advisors: Dr. Javier Segurado and Prof. Ignacio Romero
Date of defense: December 2019

13. *"High throughput screening of strength and creep properties in Mg-Zn alloys"*
Student: Na Li
Technical University of Madrid
Advisors: Dr. Jon Molina and Dr. Yuwen Cui
Date of defense: December 2019

14. *"Design, manufacture and evaluation of partially-cured composite materials"*
Student: Vanesa Martínez
Carlos III University of Madrid
Advisors: Prof. Carlos González and Dr. Juan Pedro Fernández
Date of defense: December 2019

Master/Bachelor Theses

1. *"Structural and micromechanical analysis of carbon nanotube fibres"*
Student: María Vélez
Carlos III University of Madrid
Advisor: Dr. Juan J. Vilatela
Date of defense: June 2019

2. *"New approaches for polymer electrolytes in LECs"*
Student: Luca Cabinato
University of Turin
Advisors: Dr. Rubén Costa and Dr. Carolina Barolo
Date of defense: October 2019

3. *"Water based solar cells based on SQ dyes"*
Student: Sara Ferrara
University of Turin
Advisors: Dr. Rubén Costa and Dr. Carolina Barolo
Date of defense: November 2019

4. *"Low temperature tandem solar cells"*
Student: Isabel Gomez
Technical University of Madrid
Advisor: Dr. Rubén Costa
Date of defense: December 2019

5. *"Capacidad de absorción de energía y evolución microestructural de aceros avanzados de alta resistencia de fase dual sometido a impacto por caída libre"*
Student: Mario Sanchez
Technical University of Madrid
Advisors: Peikang Xia and Dr. Ilchat Sabirov
Date of defense: July 2019

6. *"Capacidad de absorción de energía y evolución microestructural del acero inoxidable AISI 304 sometido a impacto por caída libre y perforación cuasi-estática"*
   Student: Francisco Javier Canillas
   Technical University of Madrid
   Advisors: Peikang Xia and Dr. Ilchat Sabirov
   Date of defense: July 2019

7. *"Estudio de fatiga en aceros UFH"*
   Student: Carlos Chapi
   Carlos III University of Madrid
   Advisors: Miguel Valdés and Dr. Ilchat Sabirov
   Date of defense: September 2019

8. *"Efecto de las condiciones de solidificación en la microestructura de dos aleaciones Al-1%Cu solidificadas direccionalmente "*
   Student: Luis Montes
   Technical University of Madrid
   Advisor: Bárbara Bellón
   Date of defense: Septiembre 2019

9. *"Efecto de las condiciones de solidificación y de la composición en la microestructura de aleaciones binarias Al-Cu fabricadas por moldeo."*
   Student: Jesús Martinez
   Technical University of Madrid
   Advisor: Bárbara Bellón
   Date of defense: Septiembre 2019

10. *"High-throughput screening of strength and creep properties of Mg-Zn alloys"*
    Student: Na Li
    Technical University of Madrid
    Advisors: Dr. Jon Molina and Dr. Yuwen Cui
    Date of defense: December 2019

5.2. Internships / Visiting students

1. *"High velocity impact damage in composite materials: X-ray characterization"*
   Student: Iván Campuzano
   Advisor: Dr. Federico Sket
   Visiting student from: Complutense University of Madrid
   Period: January 2019 - June 2019

2. *"Low velocity impact damage in composite materials: X-ray characterization"*
   Student: Alonso Montero
   Advisor: Dr. Federico Sket
   Visiting student from: Complutense University of Madrid
   Period: January 2019 - July 2019

3. *"Tough and high temperature resistant multilayer coatings"*
   Student: Álvaro Méndez
   Advisor: Dr. Jon Molina
   Visiting student from: Nano4Energy S.L.U.
   Period: January 2019 - December 2019

4. *"Physical and computational simulations of phase transformations in steels"*
   Student: Lucia Cobian
   Advisor: Dr. Damien Tourret
   Visiting student from: Technical University of Madrid
   Period: February 2019 - August 2019

5. *"Modelling size effects in HCP polycrystals"*
   Student: Antoine Daroux
   Advisors: Dr. Sarra Haouala and Prof. Javier LLorca
   Visiting student from: Ecole Centrale Nantes
   Period: April 2019 - August 2019

6. *"Gas atomization and laser selective melting optimization of advanced materials"*
   Student: Guo Yinuo
   Advisor: Dr. Srdjan Milenkovic
   Visiting student from: Technical University of Madrid
   Period: June 2019 - January 2020

7. *"Smart manufacturing of advanced materials"*
   Student: Gabriel Mesas
   Advisor: Dr. Jon Molina
   Visiting student from: Technical University of Madrid
   Period: July 2019 - October 2019

8. *"Critical resolved shear stresses of hexagonal Ti from nanoindentation optimization"*
   Student: Zhuowen Zhao
   Advisor: Dr. Jon Molina
   Visiting student from: Michigan State University
   Period: July 2019 - July 2019

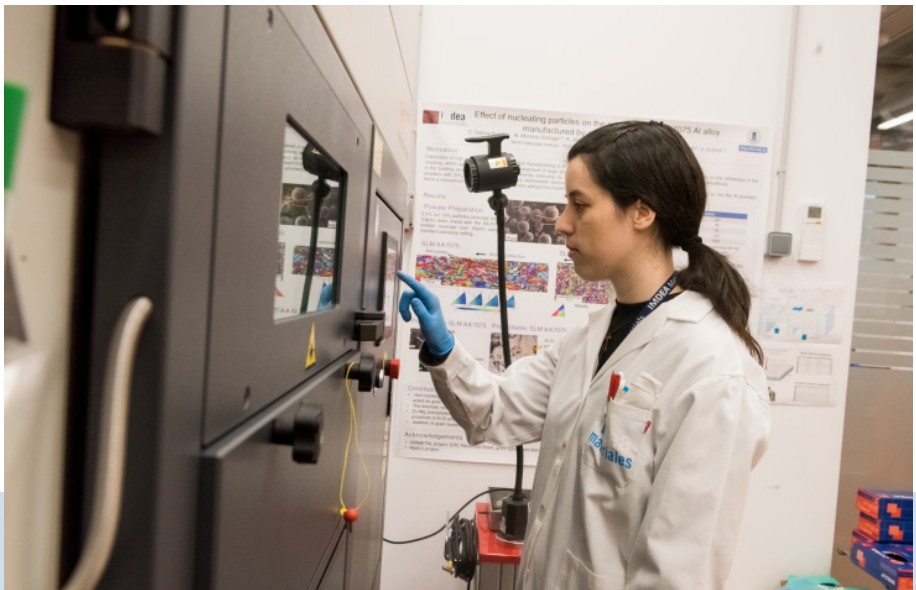
9. *"Caracterización de la unión disimilar de materiales metálicos"*
   Student: Daniel Wallerstein
   Advisor: Dr. Teresa Pérez-Prado
   Visiting student from: Vigo University
   Period: July 2019 - July 2019

10. *"Study on the manufacture and properties of mesoporous titanium oxide photoanodles"*
    Student: Isabel Gómez
    Advisor: Dr. Rubén Costa
    Visiting student from: UPM
    Period: September 2019 - December 2019

11. *"Use of ionic additives for stabilization of fluorescent proteins in polymeric media"*
    Student: Jorge González
    Advisor: Dr. Rubén Costa
    Visiting student from: Complutense University of Madrid
    Period: September 2019 - March 2020

12. *"Automatic damage analysis in 3D X-ray tomography data of low-velocity and high velocity impact of carbon fibre composite materials"*
    Student: Joaquín Bolado
    Advisor: Dr. Federico Sket
    Visiting student from: Complutense University of Madrid
    Period: October 2019 - January 2020

13. *"Dynamic mechanicl characterization of carbon fiber reinforced composites"*
    Student: Alexander Mejía
    Advisor: Dr. Federico Sket
    Visiting student from: Carlos III University of Madrid
    Period: November 2019 - February 2020



5.3. Teaching in Masters

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

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

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

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

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

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

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

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

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

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

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

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

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

14. *"Hierarchical Composites"*
    Master in Composite Materials
    Technical University of Madrid (UPM)/ AIRBUS
    Professor: Dr. Juan Jose Vilatela

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

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

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

18. *"Electrochemistry at Surfaces*"
Master in Applied Chemistry and Physics
Waseda University
Professor: Dr. Rubén Costa

19. *"Electrodepostion and Corrosion*"
Master in Advanced Science and Engineering Materials
Waseda University
Professor: Dr. Rubén Costa

5.4. Institutional activities

1. *Member of the European Materials Modelling Council (EMMC)*
2. *Member of the European Materials Characterization Council (EMCC)*
3. *Member of the European Energy Research Alliance (EERA AISBL)*
4. *Member of the European Composites, Plastics and Polymer Processing Platform (ECP4)*
5. *Local Contact Point of the EURAXESS pan-European initiative*
6. *Technical Secretariat of the Spanish Technological Platform of Advanced Materials and Nanomaterials (MATERPLAT)*
7. *Member of the Spanish Aerospace Platform (PAE)*
8. *Member of the Spanish Technological Platform for Advanced Manufacturing (MANUKET)*
9. *Member of the Madrid Aerospace Cluster (MAC)*
10. *Member of the Network of Research Laboratories of Comunidad de Madrid (REDLAB)*
11. *Member of the Spanish Railway Technological Platform (PTFE)*
12. *Member of the Spanish Energy Storage Technological Platform (BatteryPlat)*
13. *Member of the Spanish Association of Foundations (AFE)*
14. *Member of the Spanish Technological Photonics Platform (Fotónica21)*
15. *Member of the Spanish Association of Composite Materials (AEMAC)*
16. *Member of the European Aeronautics Science Network*

5.5. Individual participation in committees and other institutions

1. *Vice-President of the Spanish Association for Numerical Methods in Engineering (SEMNI). Prof. Ignacio Romero*
2. *Member of the Board of Directors of the Society of Engineering Science. Prof. Javier LLorca*

3. *Scientific Collaborator of the Carbon Hub initiative (Accelerating the Energy Transition Through Green Hydrocarbons), Rice University. Dr. Juan José Vilatela.*

4. *Honorary Adjunct Professor, Beiing University of Chemical Technology. Dr. De-Yi Wang*

5. *Fellow of Royal Society of Chemistry. Dr. De-Yi Wang*

6. *Member of TMS "Solidification" and "Young Professionals" Committees. Dr. Damien Tourret*

7. *Member of Beam Time Allocation Panel for nano-imaging and nano-analysis at the ESRF (European Synchrotron Radiation Facility). Dr. Federico Sket*

8. *Member of the Board of the Spanish Association of Composite Materials (AEMAC). Prof. Carlos González*

9. *Member of the Board of Directors of the Spanish Materials Society (SOCIEMAT). Dr. Teresa Pérez-Prado*

10. *Chair, European Mechanics of Materials Conference Committee. Prof. Javier LLorca*

11. *Member of the International Technology Advisory Board, Institut de Recherche Technologique Saint Exupéry on aeronautics, space and embedded systems, Toulouse, France. Prof. Javier LLorca*

12. *Member, Scientific Advisory Board, Manufacturing using Advanced Power Processes. EPSRC Future Manufacturing Hub, University of Sheffield, UK. Prof. Javier LLorca*

13. *Member of the Commision of the Doctoral Program on Structures, Foundation and Materials Engineering of the Technical University of Madrid. Dr. Jon Molina*

14. *Early career researcher board: IOP Multifunctional Materials. Dr. Juan José Vilatela*

15. *Scientific Committee of International Conference Carbon. Dr. Juan José Vilatela*

16. *Council Member of the International Association for Computational Mechanics (IACM). Prof. Ignacio Romero*

17. *Program Manager, Structural Materials Programme, Ministry of Innovation, Science and Universities, since 2018. Dr. Teresa Pérez-Prado*

18. *Jury member of the European MIT Innovator Awards 2019. Dr. Rubén Costa*

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

20. *Member of the Scientific Council, IRT Jules Verne, Nantes, France. Dr. Teresa Pérez-Prado*

21. *Member of the Scientific Council, NOMATEN Center of Excellence, Zwierk, Poland. Dr. Teresa Pérez-Prado*

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

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

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

5.6. Outreach

1. *Speaker at the TEDx Alcoy. "Los LEDs de nuestros nietos". March 2019. Dr. R. Costa.*

2. *Participation in the "Fair for Science and Innovation 2019" in IFEMA, Madrid, promoted by Fundación Madrid+d.* March 2019. Dr. J. P. Fernández, Dr. D. Tourret, Dr. D. Cintora, Dr. J.J. Vilatela, A. Rodríguez, V. Fernández-Luna, Dr. J. Múgica, A. Doñoro, Dr. C. Pascual, J. de la Vega, A. Fernández, J. Castro, Dr. A. García-Junceda.

3. *Speaker and panelist at the MSCA-IF Info-day at CSIC.* May 2019. Dr. D. Tourret.

4. *Participation in the STEM program of the Madrid Regional Government for mentoring of schools.* July 2019. Dr. R. Costa.

5. *Participation in the "European Researchers' night Madrid 2019", promoted by Fundación Madri+d.* September 2019. Dr. A. León, J. Fernández

6. *Speaker at the "Women in 3D printing" Madrid chapter visit at IMDEA Materials.* October 2019. Dr. D. Tourret.

7. *Participation in the "Science Week Madrid 2019", promoted by Fundación Madri+d.* November 2019. Dr. D. Tourret, C. Galera, R. Santos, Dr. J. Fernández, Dr. A. Mikhalchan, Dr. M. Vila, L. Arévalo.

8. *Organisation of primary-secondary school and bachelor-master students visits to IMDEA Materials Institute,* 8 visits during 2019 (over 250 students)

5.7. IMDEA Materials in the media

1. *Materiales 'a la carta' gracias a la nanotecnología.* Dr. J.J. Vilatela. El Mundo
2. *Energy storage in multifunctional carbon fiber composites.* Dr. J.J. Vilatela. Composites World
3. *La científica española que quiere hacer frente al reto del agua.* Dr. C. Santos. Mujeres a seguir
4. *Radio Nacional Las Mañanas, interview to Dr. C. Santos.* RNE
5. *Cleis Santos, la joven científica madrileña que sueña con agua limpia.* Retema
6. *CROR Engine Debris Impact SHielding. Design, manufacturing, simulation and Impact test preparation.* Dr. C. Lopes. CORDIS
7. *"Los jóvenes no somos unos ni-ni, sabemos hacer cosas importantes y somos el futuro", interview to A. Fenández (Premio Nacional de Juventud en Medio Ambiente).* Diario 16
8. *El investigador que trabaja para que tengas una bombilla Bioled en casa.* Dr. R. Costa. El Confidencial
9. IMDEA Materiales: competitividad a través del conocimiento avanzado. Madridiario
10. *Javier Llorca, primer español elegido fellow por la asociación de ciencia de materiales más importante del mundo.* Notiweb, Madri+d
11. *El Instituto IMDEA Materiales lidera un proyecto de impresión 3D para el desarrollo de la industria 4.0.* Dr. J. Molina. Notiweb, Madri+d
12. *En route to "massless energy" with structural power composites.* Dr. J.J. Vilatela. JEC Composite World.
13. *Un antídoto contra la sangría de 'cerebros' españoles.* Dr. R. Costa. El Mundo
14. *Radio Nacional Las Mañanas, interview to Dr. R. Costa.* RNE.
15. *Telediario de Antena 3, interview to Dr. R. Costa.* Antena 3
16. *Futuro es apasionante.* Dr. R. Costa. Vodafone El Pais
17. ¿Puede ser peligrosa la luz *azul?.* Dr. R. Costa. Muy Interesante
18. *Innovation MIT, interview to Dr. R. Costa.* MIT
19. *Nuevos materiales que revolucionan el mundo.* Dr. T. Pérez-Prado. El Mundo
20. *La española que quiere imprimir el motor de un avión en 3D.* Dr. T. Pérez-Prado. El Mundo
21. *3-D printed lattices mimic crystalline materials for extra strength, interview to Dr. T. Pérez-Prado.* Chemical Engineering News
22. *Materiales, interview to Dr. T. Pérez-Prado.* El Mundo, Extra Innovación
23. *Making plastics less flammable.* Dr. D.Y. Wang. Physics world

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