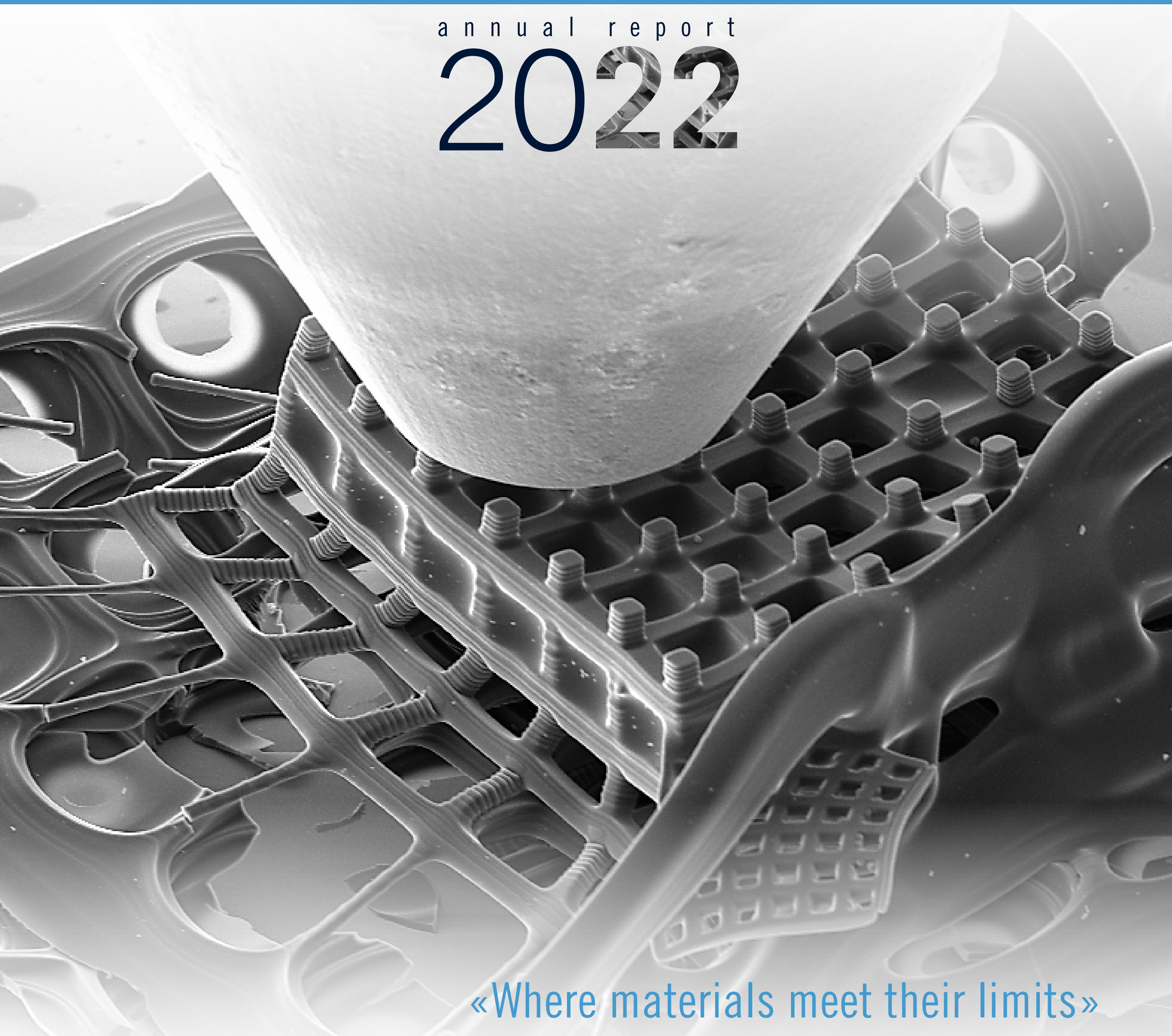
institute imdea materials

www.materials.imdea.org

annual report

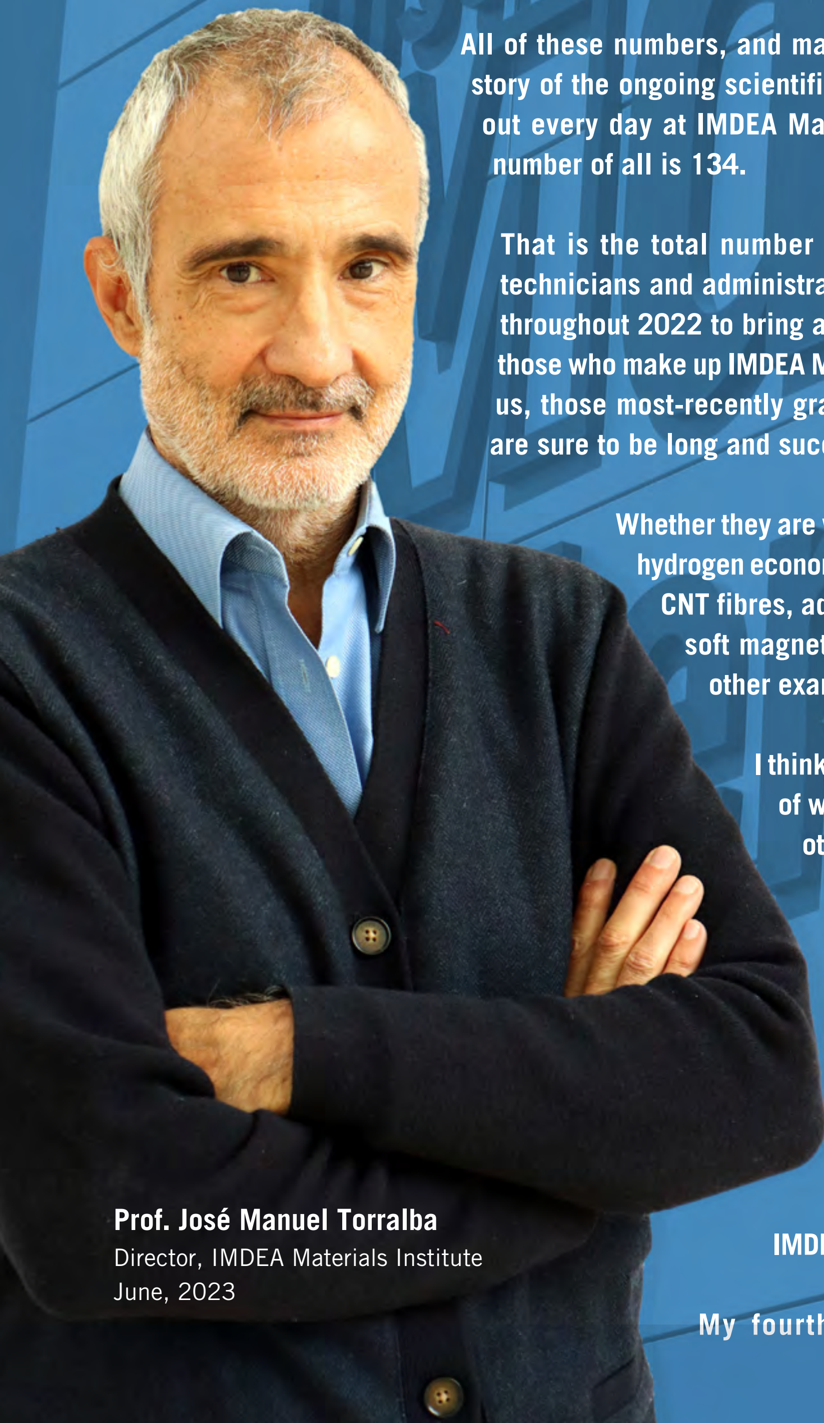
2022



«Where materials meet their limits»

WORDS FROM THE DIRECTOR...

When speaking about IMDEA Materials in 2022, let's start with some figures. 30: the number of new projects granted to the Institute in the past twelve months. 17: the number of new fellowships awarded to our researchers. 138 articles published, and 7279 citations, a new record. 64 active research projects, 61 active Ph.D. theses, 5 patent applications...



Prof. José Manuel Torralba
Director, IMDEA Materials Institute
June, 2023

All of these numbers, and many more that I haven't mentioned, tell a story of the ongoing scientific excellence and research being carried out every day at IMDEA Materials. But perhaps the most important number of all is 134.

That is the total number of IMDEA Materials staff, researchers, technicians and administration, all of whom continued to work hard throughout 2022 to bring about positive change. When I think about those who make up IMDEA Materials, I think about the youngest among us, those most-recently graduated who are just setting out on what are sure to be long and successful careers in science and research.

Whether they are working on designing new catalysts for the hydrogen economy, high-performance composites based on CNT fibres, additive manufacturing breakthroughs, new soft magnetic materiales, or immersed in countless other examples of cutting-edge scientific research.

I think about our postdoctoral researchers, some of whom have been with us for many years, or other, new faces who only joined us in 2022, but who are already making their mark on the Institute.

Our incredible technicians, who somehow find the time to not only conduct research excellence of their own, but who are also on hand to assist the entire staff in taking advantage of the incredible facilities on offer here at IMDEA Materials.

My fourth-floor colleagues, those in project management and administration who keep everything running behind the scenes, whose work may not often be highlighted, but which is undoubtedly invaluable.

And last, but certainly not least, my fellow group leaders and senior researchers, without whose tireless patience and dedication, none of the incredible research being done in such a wide variety of fields, in novel materials and advanced manufacturing, in simulation and characterisation, or in machine learning and artificial intelligence, would be possible.

Bringing the best people from all four corners of the globe to IMDEA Materials has always been, and always will be, one of the three pillars of our mission. And the diversity of our staff, representing more than 24 countries, a number which continues to grow year after year, is evidence of that commitment.

In 2022, IMDEA Materials celebrated its 15th anniversary. And it is only thanks to the tremendous work that I have just mentioned that our reputation as a centre of scientific excellence continues to grow. I am proud to say that we are a María de Maeztu Centre of Excellence, an honour awarded by the Spanish State Research Agency.

It would be impossible to mention all the Institute's new research projects which have made their mark in the past 12 months.

But whether they are focused on creating a new generation of bioabsorbable implants like BIOMET4D, leading innovation in the field of additive manufacturing like CONSTRUCTADD or PORMETALOMICS, or investigating materials which could help to play a part in ushering in a new age of nuclear fusion reactors, like MENAWIR, they are all central to our second mission, to do science of excellence.

Many of these projects involve close collaboration with our many industrial partners, and we continue to deliver on the third pillar of our mission as a scientific institute, to transfer technology to industry and to society where its impact will be most felt.

It need not be said that the past few years have been difficult, and continue to be so, for many of us. 2022 was no different. While a worldwide pandemic slowly faded from the headlines, Europe was once again plunged into war.

And yet, in my second year as Director of IMDEA Materials, as someone who sees the very best of endeavour and discovery, of hard work and dedication every day within the halls of this Institute, I am more convinced than ever that a bright future lies ahead in 2023, and beyond.

annual report

2022

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editor

IMDEA Materials Institute

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Dr. Miguel Monclús. Winner imaging contest 2022. Materials Characterisation and Public Choice.

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About us

IMDEA Materials Institute, one of seven Madrid Institutes for Advanced Studies (IMDEA), is a public research centre founded in 2007 by Madrid's regional government. The Institute's goal is to carry out research at the forefront of Materials Science and Engineering, to attract talent from around the world, and to collaborate with companies to transfer fundamental and applied knowledge into valuable technology.

...RESEARCH PROGRAMMES

Novel Materials

Integrated Computational Materials Engineering

Advanced Manufacturing

Multiscale Characterisation of Materials and Processes

Our...

...mission

Research of excellence in Materials Science to tackle the challenges facing society and to foster the sustainable development of the Madrid region.

...vision

To continue enhancing IMDEA Materials' reputation as a leading research institute, one which is internationally recognised for its excellence in Materials Science and its contributions to the positive transformation of society.

...facilities

IMDEA Materials Institute is located in the Scientific and Tecnological Park of the Technical University of Madrid in Tecnogetafe, Madrid, Spain.

Our 2,640 m^2 of state-of-the-art laboratories offer the capacity to manufacture, characterise and simulate advanced materials and nanomaterials, including their integration in lab-scale prototypes and devices. The Institute also boasts a 200-person auditorium and networking space for international conferences and workshops.

...technology

Metals, composites, polymers, 3D printing, multiscale modelling and artificial intelligence, nanostructured materials, multiscale characterisation of materials and processes, fire resistance, electrochemistry and biomaterials and cell culture.

...SECTORS AND AREAS OF APPLICATION

...people

The core strength of IMDEA Materials is our people. The Institute's international research team consists of 100 talented researchers from 24 different countries, realises scientific discoveries in Materials Science, and fosters the development of emerging technologies.

We continue to focus on the implementation of our Gender Equality Plan which seeks to increase the number of seminars given by women by 10%, and to increase the participation of women on our Scientific Council and Industrial Advisory Board so that their composition reflects that of the Institute's current staff.

IMDEA Materials already boasts a percentage of female researchers far above the average for the engineering and technology sectors and the overall percentage of women among the Institute's ranks continues to increase each year. We are also recognised as a centre of Human Resources Excellence in Research by the European Commission. IMDEA Materials has held this distinction since 2015 and is committed to providing the most attractive and welcoming environment for researchers and staff.

An internal survey conducted in March 2022 in relation to this area found that an overwhelming majority (85%) of IMDEA Materials staff believe that the Institute's commitment to improving employee health and wellbeing has increased in recent years and the general engagement index that measures commitment and pride in belonging to the Institute is 90%.

The same survey also found that awareness of the ethical and professional aspects of their roles is also very high among researchers and that there is a general perception of professional fulfilment at work.

100
Researchers

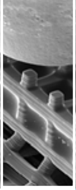
58%
Foreign Researchers

37%
PHDS

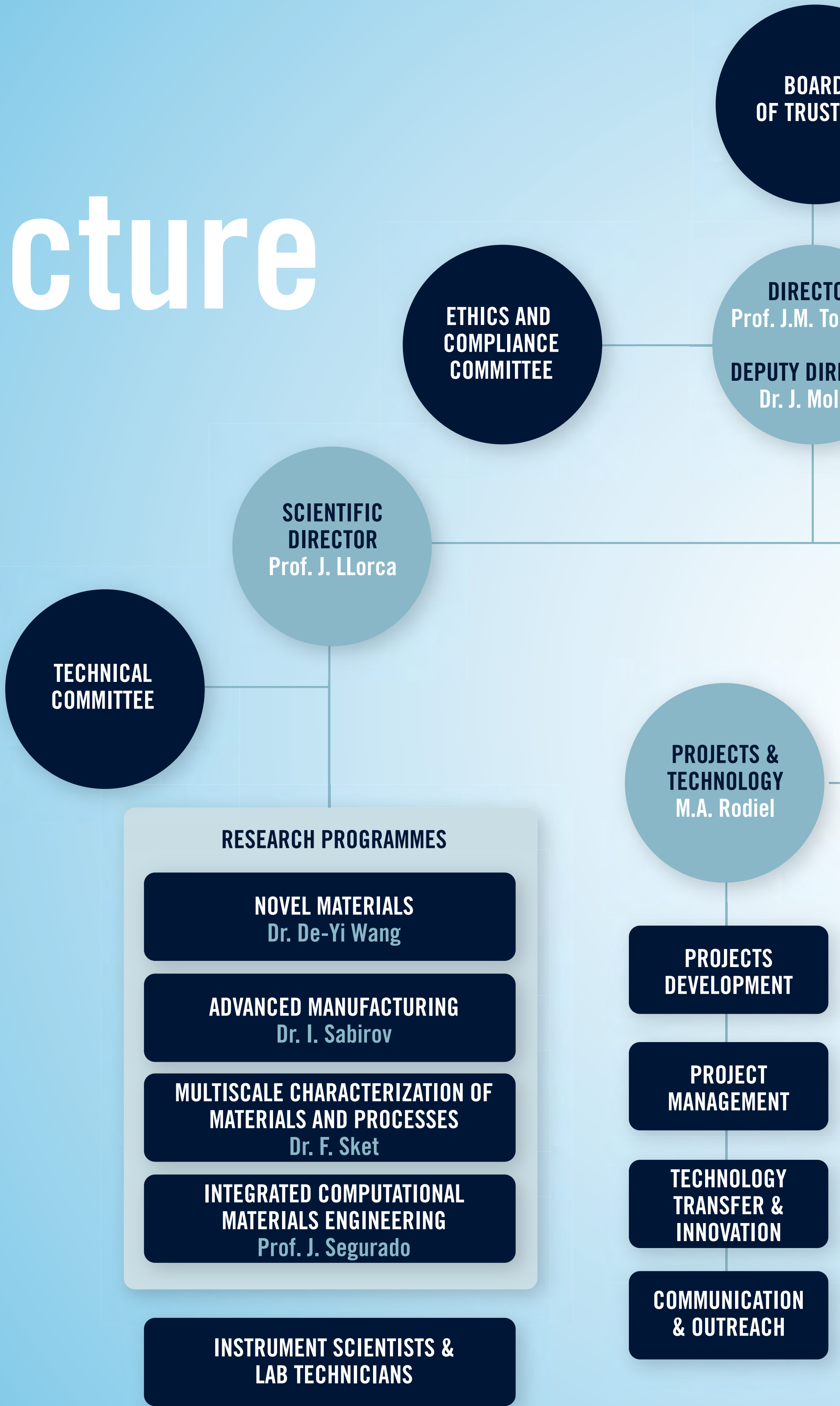
24
Nationalities

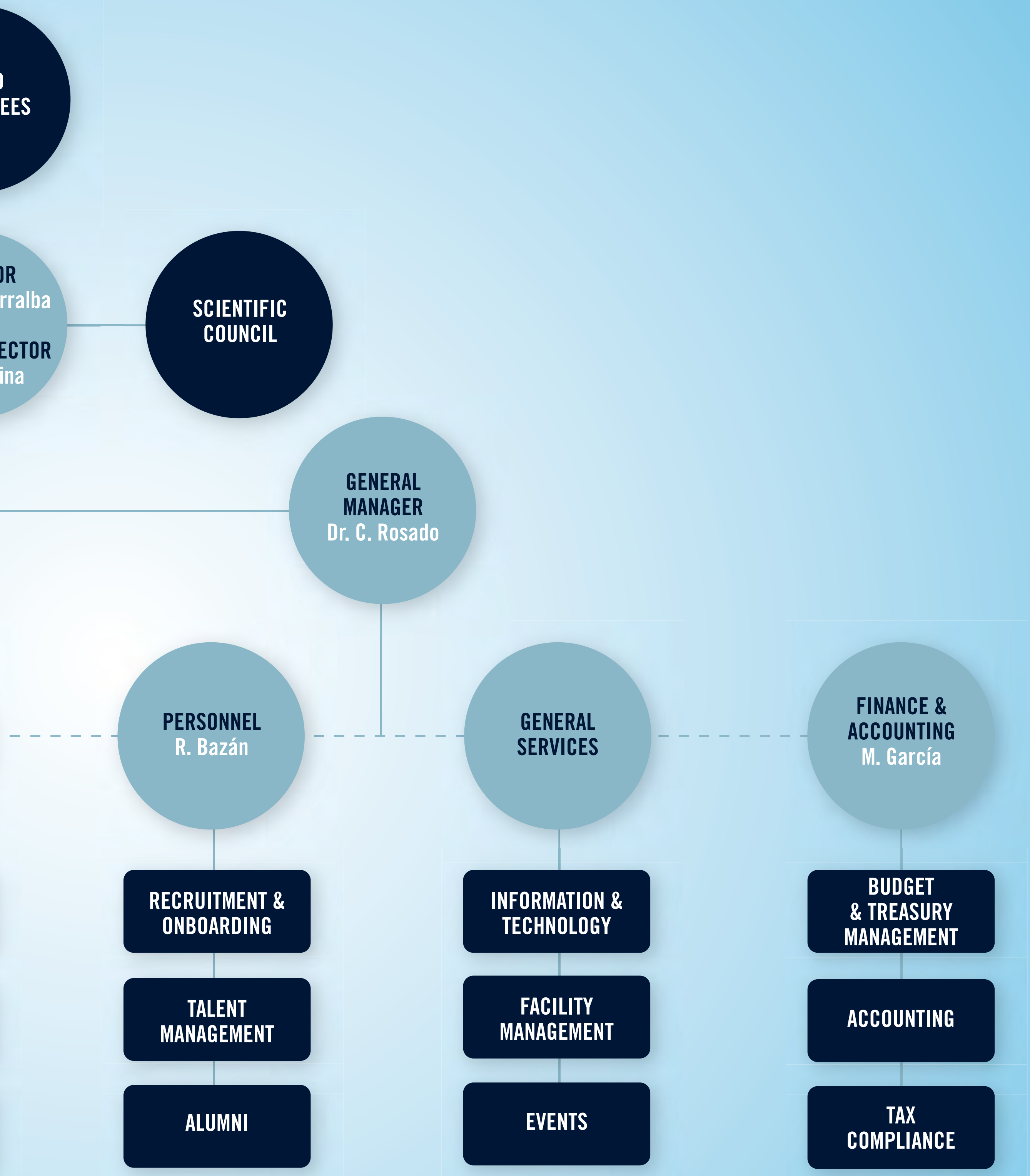
30%
Female researchers

16
Research groups



our structure

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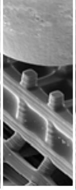

our structure

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in figures

human resources

talent

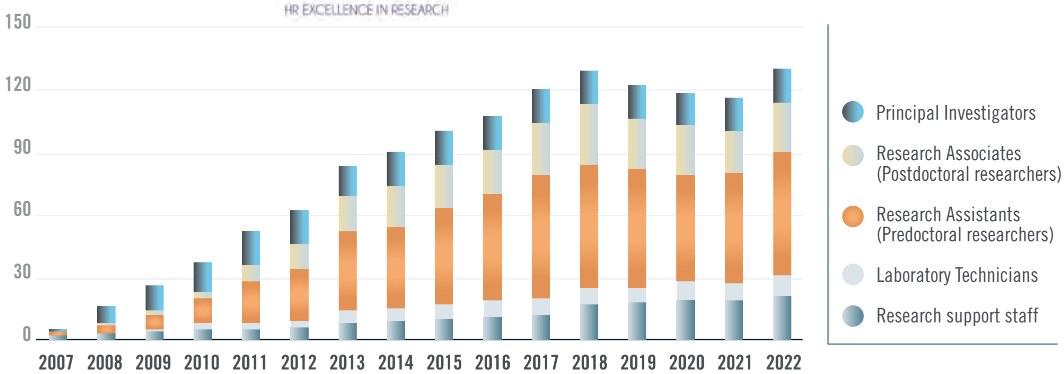
Talent attraction has been the key to the Institute's **success**.

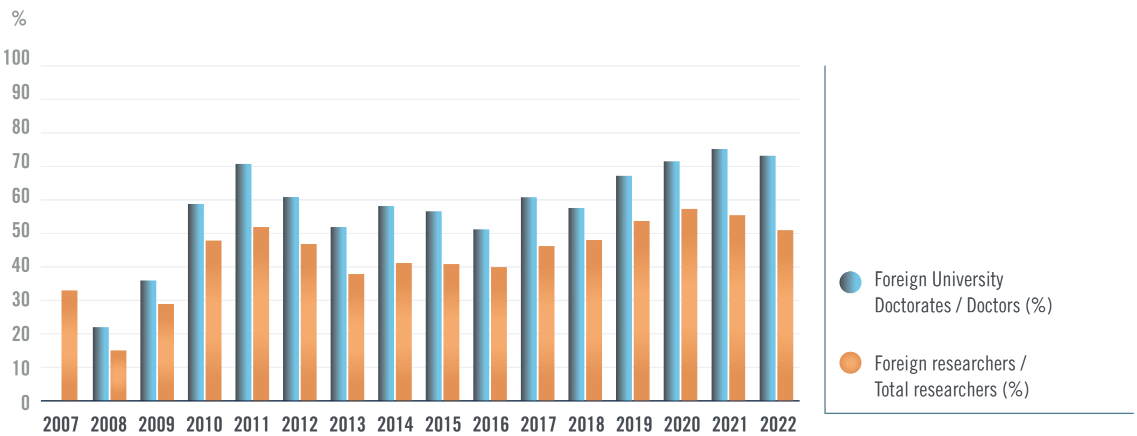
An open and transparent selection process along with regular evaluations performed by an independed Scientific Council ensures the excellence of our Principal Investigators.

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.

HR EXCELLENCE IN RESEARCH





Technology and knowledge transfer to society through **talent transfer**

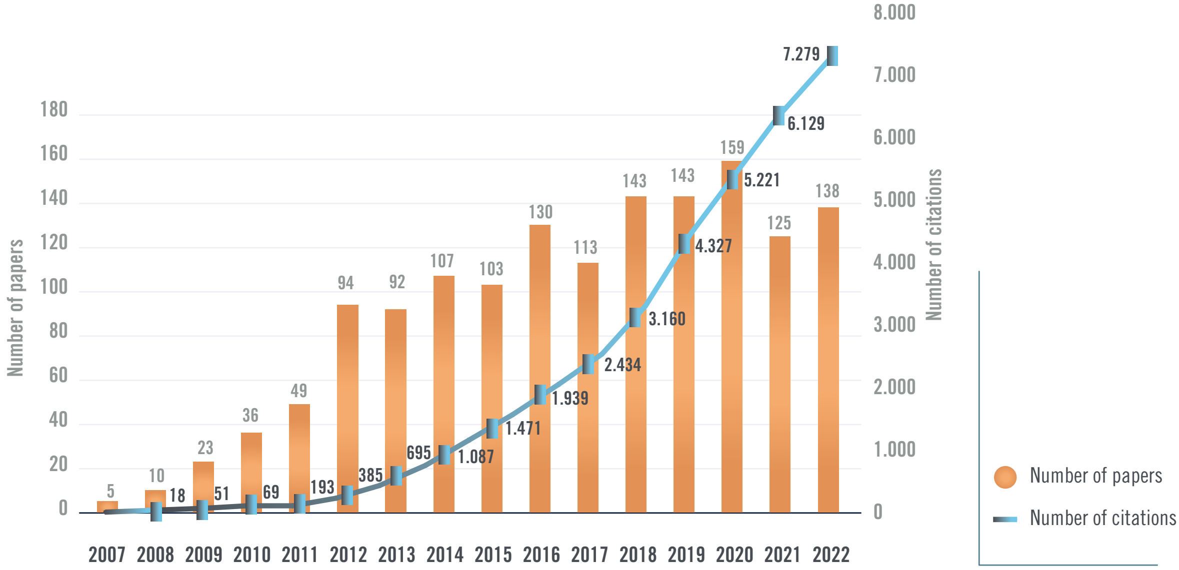
89 Defended PhD theses since 2007

55 Ongoing PhD theses

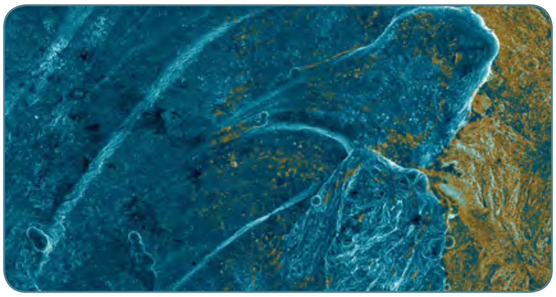
scientific results

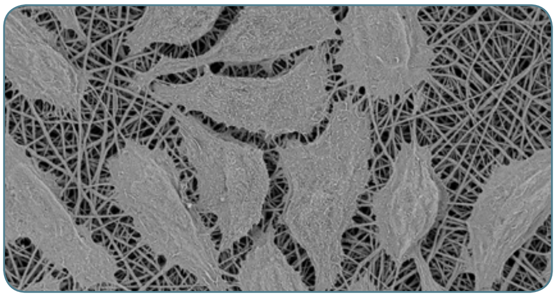
science

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



2022





40 Keynote/ invited talks

138 Papers (SCOPUS)

7279 Citations (SCOPUS)

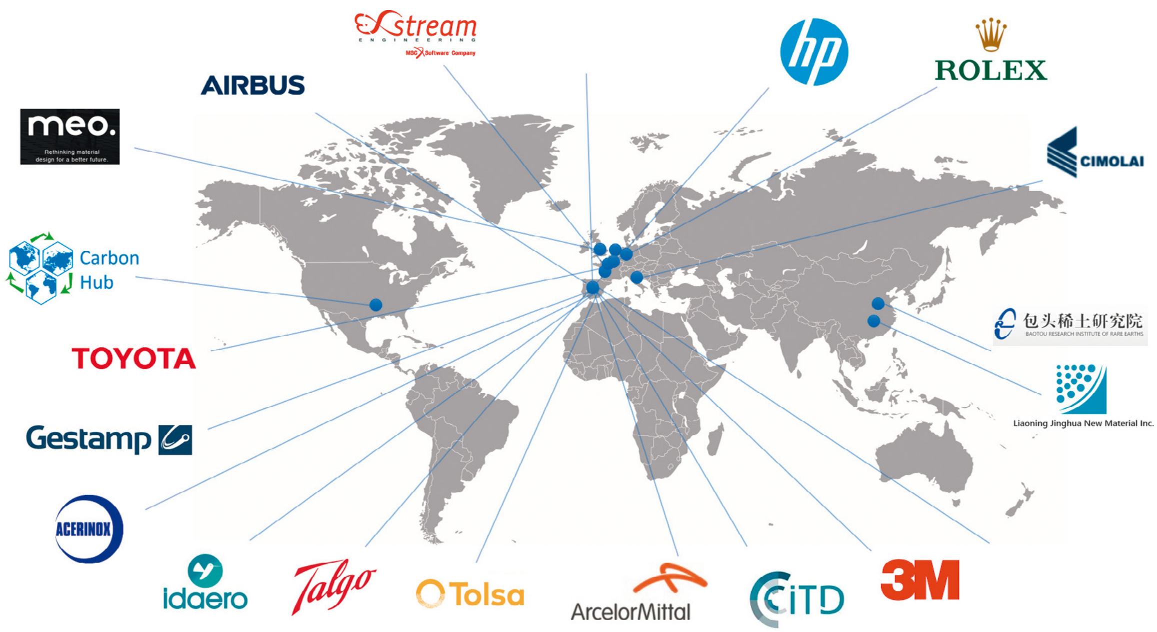
12 Invited seminars and lectures

technology transfer and innovation

transfer

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

Companies which had active collaborations with the IMDEA Materials Institute in 2022:



Performance indicators in 2022

10
New bilateral projects with industry

2
Industrial Doctorates

5
Patent applications

14
Patents in portfolio (granted and under evaluation)

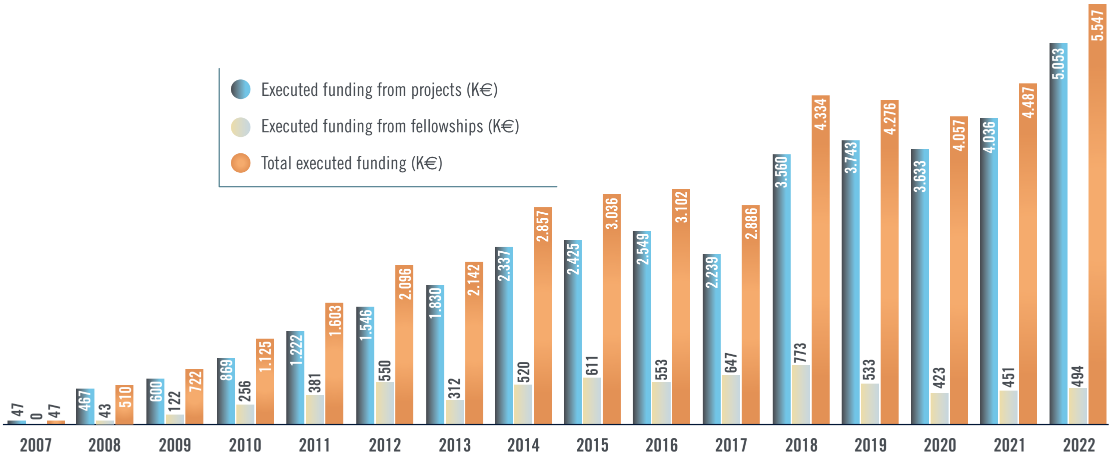
1
Patents licensed

7
Software tools licenses

1
Spin-offs:
(FLOATECH, S.L.)
Floatech®

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.



2022

International projects
23%

National projects
20%

Regional projects
45%

Contracts with industry
12%

64
R&D projects

2
Active ERC projects

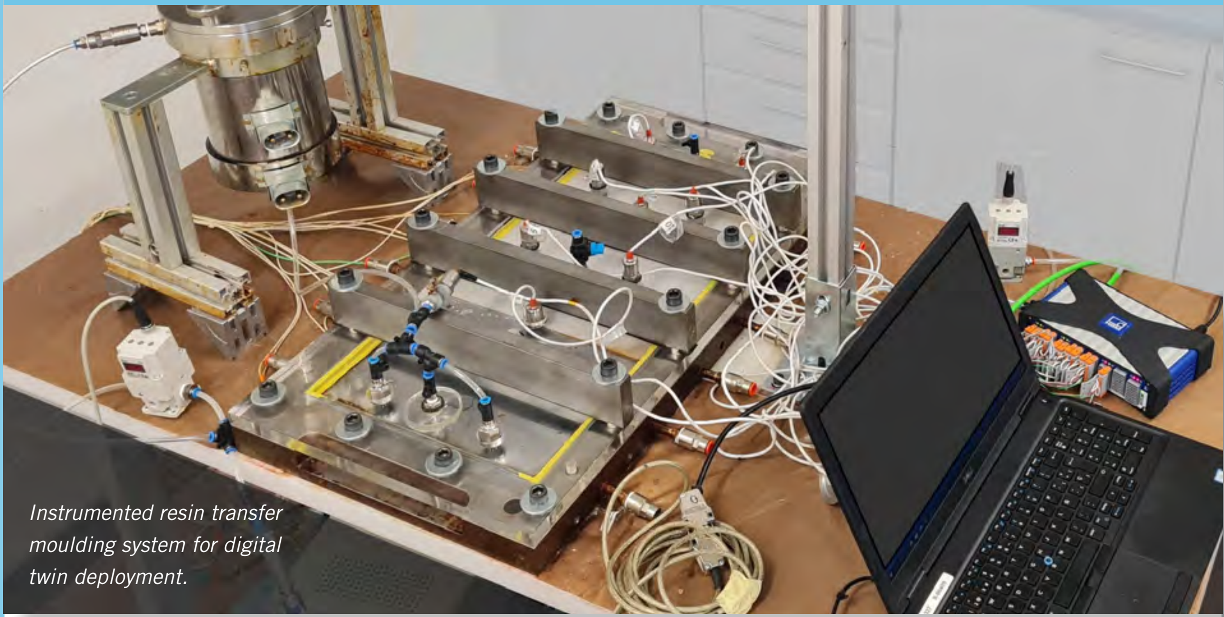
3
Active FET-OPEN / EIC Pathfinder Open projects

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



Instrumented resin transfer moulding system for digital twin deployment.

Metallic alloys

- Bulk processing techniques: induction casting 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, instrumented resin transfer moulding for digital twin deployment, VI vacuum infusion, RFI resin film infusion and pultrusion, prepreg lamination using vacuum bagging of autoclave and out-of-autocave prepregs (OoA) or laminate hot-press moulding (<400°C). Semi-industrial equipment for compounding (microcompounder and twin two-screw extruder) and injection moulding (industrial injector and mini-injector machine) of thermoplastics, integration of advanced nano-fillers, filament maker for 3D printing (3dvo) and melt flow index.

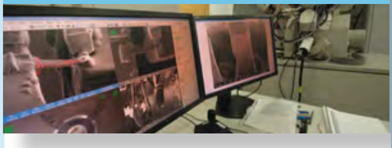
Nanomaterials

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

Energy storage and conversion devices

- Synthesis and characterisation of nanostructured electrode materials for energy storage. Fabrication of composite electrodes and intergration in rechargable batteries (Li-ion, Li-S, Li-02, Na-ion, hybrid etc.). Fabrication and testing of nanocarbon-based electrodes and their integration with liquid and solid electrolytes to form large-age (>100 cm2) flexible supercapacitors. Integration of energy-storage functions in structural composites. Fabrication (solvent-based deposition), physical vapour deposition, high-temperature sintering overs and hot plates and characterisation. Fire-testing devices for electrolites and in situ XRD device for battery applications.

Microstructural and chemical characterisation

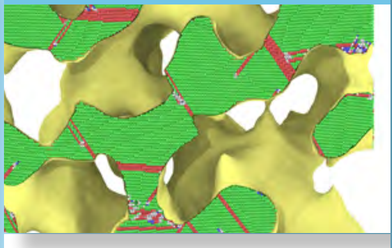


- 3D microscopy at different length-scales, including X-ray tomography, X-ray diffraction, 3D-SEM, 3D-EDS and 3D-EBSD in the FIB, and 3D-TEM and 3D-EDS in the TEM.
- In-situ thermos-mechanical testing of miniaturised samples in the X-ray tomography system, as well as in the SEM and TEM.
- In-situ processing studies in the X-ray tomography system, such as casting, infiltration and curing of polymer based materials.
- Raman spectrophotometer and Gel permeation chromatography.
- Particle size analyser, freeze dryer and in-situ thermal studies of polymers in the X-ray diffractometer.
- In-situ termal studies of polymer in X-Ray diffractometer (SAXS/WAXS).
- C-Scan ultrasound non-destructive inspection system.

Mechanical Properties

- Mechanical materials testing, using electromechanical and hydraulic machines (quasi-static, dynamic, fracture and fatigue testing in a range of temperatures).
- Mechanical property characterisation at multiple length scales, including nanoindentation, micropillar compression, microtensile testing and microfracture mechanics.
- Tests can be carried our both ex-situ and in-situ in SEM, TEM and X-ray tomography including measurements at elevated temperatures.
- Tensile tests can be carried out in-situ in dual cone calorimetry.

Simulation



- Simulation techniques at different scales (electronic, atomistic, mesoscopic and continuum), to design or improve materials and components by means of virtual testing and processing.
- High performance computer cluster (600+ Intel Xeon CPU cores and NVIDIA GPU accelerating leading to a computational power of 90 Tflops)
- In-house developed simulation tools including Iris, Muesli, FFTMAD, CAPSUL, etc. as well as commercial and open source software tools for modelling and simulation in Materials Science and Engineering (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 UL9F Horizontal/ Vertical Flame Chamber.

Thermal

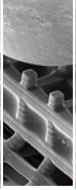
- DSC, TGA and Hot Disk Thermal Conductivity analyser. Thermal behaviour of mechanical properties, DMA and rheology.
- Pushrod Dilatomer to measure dimensional changes.

Electrochemical

- Electrochemical characterisation of energy storage devices (Li-ion, Li-S, Li-02, Na-ion and hybrid batteries). Simultaneous testing of 100 batteries can be performed using multichanel battery testers.
- Galvanostatic/potentiostatic cycling at various current densities.
- Single channel Zive SP1 electrochemical workstation for cyclic voltammetry (CV) and electrochemical impedance spectrocropy (EIS) study of batteries.
- LCR equipment to quantify dielectric properties in composites.

Biomaterials and cell culture

- Confocal, fluorescence, and brightfield microscopes.
- PCR instrument, multi-mode plate reader, ultrasonic processor, lyophilizer, autoclave, Spectrofluorometer and dynamic light scattering equipment.
- Microfluidic system, gel electrophoresis and blotting system.
- Liquid nitrogen tank for cell storage and -80C freezer.
- Prusa Mini 3D printer and Phrozen Sonic Mini 8K resin 3D printer.
- Biosafety cabinets, benchtop and CO2 incubators.
- Centrifuge, microcentrifuges, vortex mixers, pipet controllers, hot plate stirrers, dry block heaters, UV lamps, pH meter, balance, and thermostatic water baths.



research programmes

talent

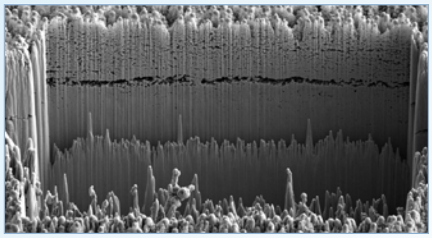
science

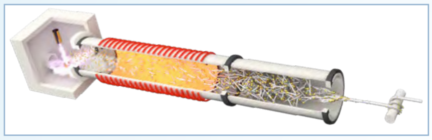
transfer

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.

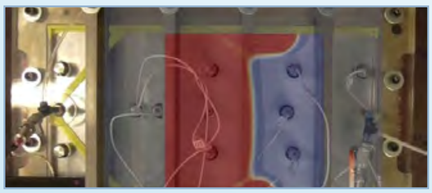
As a result of a high degree of internal collaboration, each research group at the IMDEA Materials Institute participates in several of our **research programmes**. Driven by the talent of the researchers, the research programmes combine cutting-edge fundamental oriented research in topics at the frontiers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

Advanced Manufacturing

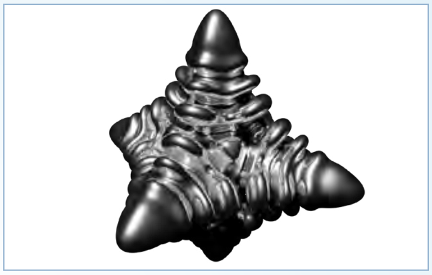




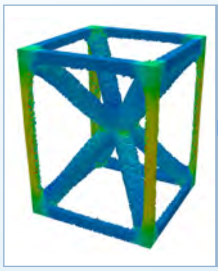
- Industry 4.0 and the virtual testing of structural materials.
- AI techniques applied to manufacturing and AI-guided materials design and chemical process.
- Bulk nanostructured materials: gas-phase assembly of continuous fabrics and fibres of CNT nanotubes and inorganic nanowires.
- Liquid and solid-state processing.
- 3D printing of metallic materials, composites, polymers, recycled fibres and hybrids. Data-driven design of 3D-printed metamaterials, predicitive simulation, in-situ monitoring etc.

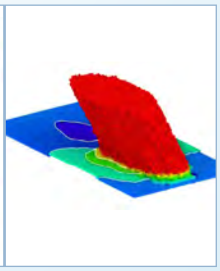


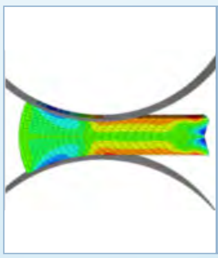
Integrated Computational Materials Engineering



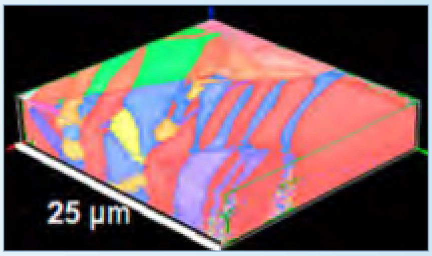
- Virtual materials design, including virtual processing and virtual testing
- Materials modelling at different length and time scales
- Multiscale materials modelling
- Modelling and simulation strategies for different applications
- Computational and data-driven materials discovery



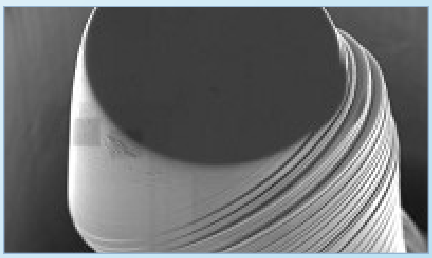




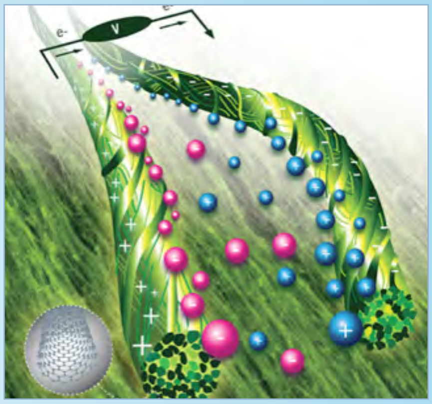
Multiscale Characterisation of Materials and Processes



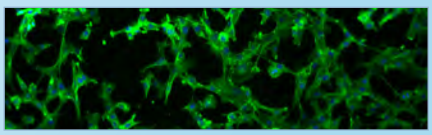
- Advanced material characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques
- 4D characterisation: in-situ multiscale characterisation of processes
- Correlation between experiments and multiscale simulations (molecular dynamics, dislocation dynamics, crystal plasticity, finite elements,...)



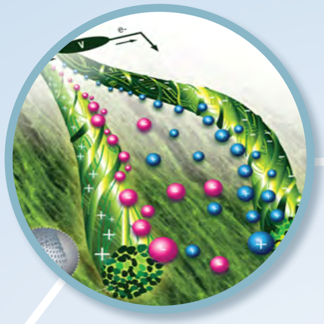
Novel Materials



- Synthesis and integration of nanomaterials (nanotubes, nanowires, ninofibres MXene, 2D nanofillers etc.)
- Synthesis and properties of polymer-based multifunctional nanocomposites
- Materials for the hydrogen economy
- Metallic materials
- Structural composites
- Materials for extreme conditions
- Materials for Lithium-Ion Batteries (LIBs) and materials for post LIBs
- Green and lightweight materials approaches
- Regenerative engineering and medical treatments



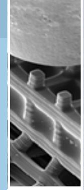
programme
Novel Materials



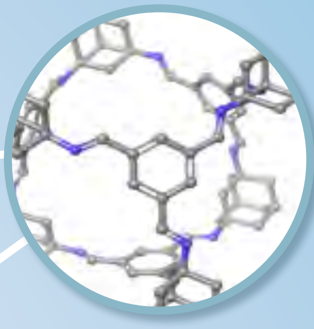
Multifunctional Nanocomposites

Goal and vision

The Novel Materials programme combines expertise in design and synthesis of nano and molecular building blocks with their integration into macroscopic materials and devices to develop solutions for high-performance structural composites with enhanced multifunctional capabilities such as thermal, electrical and fire resistance, and in exploring 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 chemists, physicists, and engineers (chemistry, materials, mechanical and aeronautical) carrying out both fundamental and applied research via close collaboration with companies in the transport, aerospace, energy, safety, and biomedical sectors. Research facilities include state-of-the-art equipment for synthesis, processing, manufacturing, structural/materials characterization and material properties.



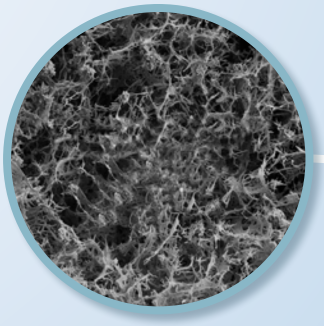
High Performance Polymer Nanocomposites



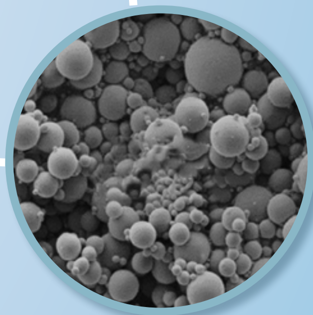
Computational and Data-Driven Materials Discovery

Structural composites

Nanomechanics and Micromechanics



Biomaterials and Regenerative Medicine



Sustainable Powder Metallurgy

Main research lines

Synthesis and integration of nanomaterials (nanotubes, nanofibers, MXene, 2D nanofillers, etc.)

- Synthesis of nanocarbon/semiconductor hybrids for photo and electrocatalysis, interaction of nanocarbons with liquid molecules, polyelectrolytes and inorganic salts.
- Synthesis of inorganic nanowires and assembly as macroscopic yarns and fabrics.
- Sensors: triboelectric, thermoresistive chemical, piezoresistive, piezoelectric.
- Hierarchical materials: materials design from the nanoscale to the macroscale, nano-reinforced materials, composite materials with enhanced electrical and thermal conductivity.
- Electrospinning for polymeric nano-membranes.

Synthesis and properties of polymer-based multifunctional nanocomposites

- Sustainable materials: bio-based nanocarriers, novel guest-host nanomaterials, nano-cross linkers, multifunctional polymer nanocomposites, renewable and recyclable polymeric materials, biodegradable polymers, carbon fiber reinforcement, etc.
- Fire retardant materials through nanodesign: multifunctional nanomaterials to increase fire retardancy: layered double hydroxides, Metal-Organic Framework, sepiolite, molybdenum disulphide, nanocarbon, nano metal hydroxide, graphene, cellulose nanocrystal, etc.
- Energy storage and energy saving materials.
- Phase-change materials for thermal management.

Materials for hydrogen economy

- High-throughput design and synthesis (magnetron sputtering) of novel catalysts for green hydrogen production and energy generation from hydrogen by means of elastic strain engineering.
- Development of new metallic alloys to be used in hydrogen embrittlement conditions.

Metallic materials

- Advanced high-strength steels showing a combination of enhanced mechanical and in use properties.
- High alloy steels, superalloys and high entropy alloys.
- Analysis of chemistry-processing-microstructure-properties relationship on macro- and microscales with emphasis on their strength, ductility, fatigue and fracture resistance.
- Study of solidification-microstructure relationships using traditional (vacuum induction melting, vacuum arc melting, gravity and tilt casting, directional solidification) and advanced techniques (centrifugal and suction casting, vacuum melt atomization).
- Rapid screening of phases, crystal structures, properties, microstructure and kinetics in bulk materials by the Kinetic Diffusion Multiple Technique.
- Deposition of multiscale functional coating layer by employing methods such as blade casting, spin coating, spray coating, electrospining, etc.
- Structural-mechanical property relationships for lightweight porous metal structures.

Structural composites

- Manufacturing of structural composites by liquid moulding (resin transfer moulding and vacuum infusion) and autoclave consolidation. Additive manufacturing of fibre reinforced composites.
- Material design for damage tolerant and impact resistance applications including multimaterial integration.
- Hierarchical integration of nano filler reinforcements for damage tolerant, electrical, lightning impact applications.
- Recycling techniques for polymer-based composites.

Materials for extreme conditions

- Impact, high temperature, mechanical, fire, predictive simulation.
- Predicition and prevention strategy for metal, polymer based composite materials under simutaneouly extreme condicitons such as high temperature behavior under structual loading.
- Alloys to be used at high temperature and corrosive environments.

Materials for Lithium-Ion Batteries (LIBs)

- Nanostructured silicon anodes.
- Carbon nanotube fabrics for hybrid electrodes and metal-free current collectors.
- Defect-engineered electrodes.
- Fire-retardant electrolytes.
- Flame resistant all solid-state polymer electrolytes.
- Electrolyte composition optimisation accelerated by Artificial Intelligence.
- Flexible and structural batteries.

Materials for post LIBs

- Fire-retardant electrolytes.
- Electrolyte composition optimisation accelerated by AI.
- New electrodes and interfacial strategies for Zinc-ion batteries.

Lightweight materials

- Composite materials.
- Alloys.
- Hybrids.
- Sandwich-structured fire retardants.
- Porous polymers and polymer-based aerogel.
- Reversible crosslinking.

Green materials approaches

- Bio-based polymers fibres and additives.
- Reprocessable composites.
- Valorization of by-products in hydrogen production.
- Biobased thermal energy storage/phase change materials.
- Development of advanced alloys avoiding the use of critical materials.

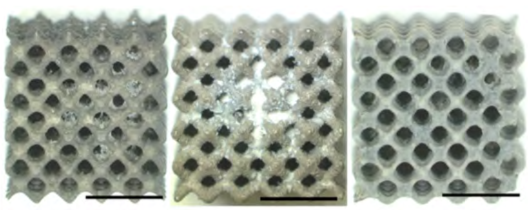
Regenerative engineering

- Bioresorbable 3D printed metallic and composite scaffolds for bone regeneration.
- New materials for tissue engineering and regenerative medicine.
- Biodegradable cardiovascular metallic stents via 3D printing.
- New materials and devices for organs-on-chips, spheroid/organoid generation, and in vitro tissue models.

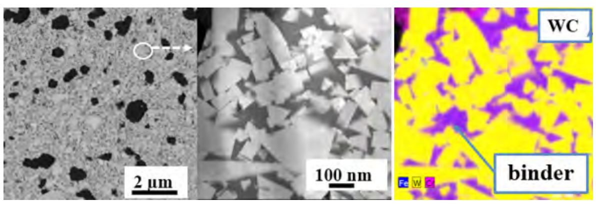
Medical treatments

- Degradable metal nanoparticles for biomedical applications (anticancer or antibacterial activity).
- Biofunctionalization and surface modification on materials with molecules to improve their performance.
- Mechanotransduction.

Screening of fire insulation properties of polymer composite panel with thermal camera



3D printed Mg scaffolds for bioresorbable bone implants



New cemented carbides Cr-Fe based nano-reinforced

Projects in focus

UNIYARNS / Universal Processing Route for High-Performance Nanostructured Yarns

European Research Council

Funding: ERC-2021-COG. European Research Council Executive Agency (ERCEA)
Project coordinator: IMDEA Materials
Project period: 01/09/2022 – 31/08/2027
Principal Investigator: Dr. Juan J. Vilatela

Yarns are a natural architecture to assemble small building blocks into macroscopic objects and are thus woven into our history, from fabrics of natural fibres in ancient times to fibres of synthetic polymers developed in the 20th century for lightweight applications. Humankind's new building blocks are nanomaterials, with superlative properties in all areas (optoelectronic, catalytic, transport, structural) relevant for global challenges related to energy use, storage and conversion.

UNIYARNS proposes a new universal route for gas-phase assembly of one-dimensional nanomaterials into kilometric yarns, applicable to materials central to energy applications (metal oxides, semiconductors and semi-metals), and reaching high volume fractions without use of processing solvents or polymers.

The strategy is to grow ultra-long nanomaterials by atmospheric-pressure floating catalyst chemical vapour deposition (FCCVD) at sufficiently high concentration for them to entangle and form aerogels suspended in the gas phase that can then be directly drawn as continuous, macroscopic yarns.

The first objective of the project is to demonstrate the generality of the FCCVD synthesis process, with a particular focus on metal oxide nanowires. A further objective is to study the kinetics and reaction paths in 1D nanomaterials synthesis with floating catalysts in order to understand the exceptionally fast growth rate inherent to this synthesis mode and to explore its boundaries of selectivity and conversion.

The next objective is to describe aerogel formation by determining factors at the aerogel network level and at the molecular-scale level that govern gas-phase assembly. The final objective is to establish clear structure-property relations for nanostructured yarn systems to overcome the current envelope of materials properties through the low charge transport resistance and high toughness of their network structure.

For more information, please contact
Dr. Juan José Vilatela at juanjose.vilatela@imdea.org

Schematic representation of an FCCVD reactor for generating silicon nanowires in the gas phase (left) and a photo of a stripe of self-standing silicon nanowire fabric showing its flexibility in terms of bending and knotting.

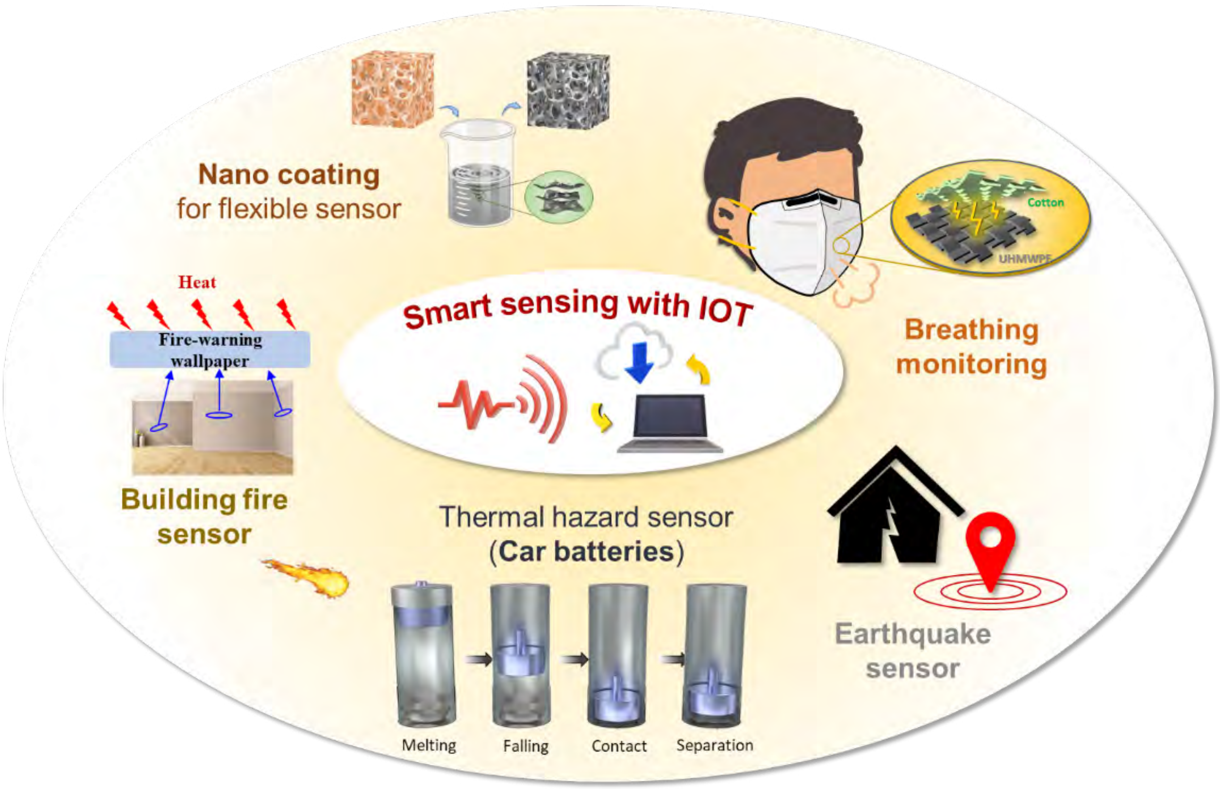
Research highlights

Smart sensing: from fire management to breating monitoring

One of the technologies that has improved every-day life in society are sensors. Sensors are capable of detecting changes in the environment and translating electrical impulses as a response.[1] These technologies are capable of sourcing different physical attributes including light, temperature, movements and pressure, and acting as a response.

In recent years, the prefix "smart" has been added to sensors thanks to technological advances: inexpensive high-resolution cameras, efficient smartphones and cheap robotics[2]. In fact, under the IoT (Internet of Things) vision, a network of smart devices could sense and transmit real-time status as a response to the state of an object, while tracking and reporting its status.

Going into detail, at IMDEA Materials over the last year, different approaches have been pursued in the field of "smart sensing", sourcing from light to temperature and even human-powered movement.



Summary of smart sensing with IOT developed at IMDEA Materials: Nano-coating for flexible sensor, Breathing monitoring, Earthquake sensor, Thermal hazard sensor and Building fire sensor.

Early detection of thermal and fire hazards: Fire warning systems

Monitoring temperature increase is a vital step to prevent fires and related fire-hazards, which cause immense damage both economically and environmentally. Especially important is monitoring temperatures at an early stage (before combustion), obtaining vital time for evacuation and prevention.

We have recently highlighted the importance of those sensors such as Early Stage Fire Warning Systems (EFWSs)[3]. EFWSs are based on a physical attribute (change of resistance) of certain materials (Graphene Oxide, GO) under reduction towards the conductive state of reduced graphene oxide (rGO).

- Novel systems based on MXene/GO/cellulose paper have been developed, with enhanced fire detection speed and warning at low temperature, 2s at 250ºC [4]. The signal is wirelessly transmitted to a liquid crystal display (LCD) screen when it displays a message such as "FIRE DANGER" which can also be sent via SMS to a mobile phone. Moreover, systems based on P/Si-Decorated Graphene Oxide were employed to design smart fire alarm paper. This paper showed a promising use as smart wallpaper for interior house decoration and other applications requiring early fire detection and warning.[5]

- Multifunctional nano-coatings with fire-warning properties were designed as a pre-designed functional solution which is wrapped into different substrates, such flexible polyurethane (FPU) foam. This illustrates the feasibility of tuning novel fire-warning nano-coating onto flammable FPU, and other materials, for fire warning systems.[5]

- Signal transmission and sensing physical attributes are as important as material choice. Therefore, other magnitudes than electrical resistance were employed to trigger EFWSs such as luminosity[6]. Signal transmission was both explored to be sent locally or remote, up to 20 km with the use of Lo-Ra [5,6] sent to a mobile phone or any other display device.

- For the first time, a self-powered thermal and fire hazard sensor was designed by coupling gravitational potential energy to the triboelectric effect to generate electric signals. Furthermore, the sensor was integrated with several communication interfaces such as a liquid crystal display (LCD), Wi-Fi emitter, light-emitting diode (LED) light, IoT network, and mobile phone. The sensor exhibited an instant response (~0 s response time) at temperature ranges between 80 and 89 °C.[7]

Triboelectric nanogenerators assisted sensing: from earthquakes to biomonitoring

Recently, Triboelectric nanogenerators (TENGs) have been designed and developed to create self-powering monitoring systems, enabled by the triboelectric voltage generated during their use. This allows harvesting energy from various sources due to movement, opening the possibility of real-time monitoring and energy-harvesting.

- New triboelectric nanogenerators employing self-powered seismic sensors (SEIS-TENGs) capable of detecting seismic waves with global connectivity to the Internet of Things (IoT).[8] SEIS-TENGs were fabricated with different materials such as Paper, Polyvinylalcohol (PVA), Polyvinyledenefluoride (PVDF) and PDMS being flame-retardant, frecuency-dependend and low cost.

- All-Fabric Textile-based TENGs (AF-TENGS) were implemented into respiratory face-masks systems (FFP2), allowing real-time monitoring of human breath. This is a first step in detecting breathing anomalies such as coughing or apnea, which can trigger an alarm system and send the information remotely.[9]

For more information, please contact
Prof Dr. De-Yi Wang at deyi.wang@imdea.org

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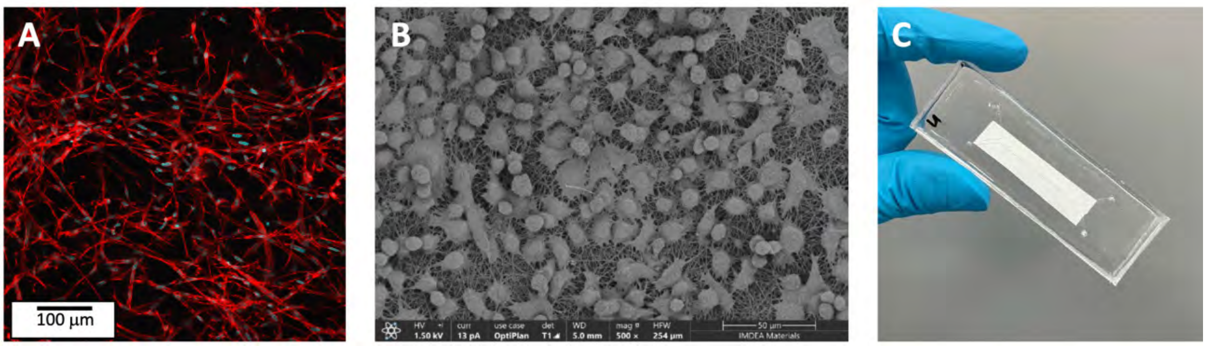
Novel material and process development for the creation of 3D in vitro models of airway and other tissues

The current global pandemic (COVID-19) and other recent major epidemics including SARS and MERS as well as the historical Spanish flu are caused by respiratory viruses that affect the lung. To better understand the pathophysiology of these diseases and develop preventive and/or therapeutic measures, translational models play a key role in the pathway towards clinical trials and range from simple cell cultures through 3D organoids to animal models. During the last decade, research into microphysiological systems, often called organ-on-chip devices or in vitro tissue models, has blossomed, including the development of lung-on-chip systems that mimic the epithelium-endothelium interface and physiological breathing movements. These devices are typically integrated into bioreactors or microfluidic circuits and further combined into high-throughput screening platforms involving data collection and analysis. Materials science plays a key role in the development of such 3D in vitro tissue models through the synthesis of biocompatible materials for use in the devices and their processing to create complex 3D geometries.

The Biomaterials and Regenerative Medicine research group at IMDEA Materials Institute is working on the development of novel materials and simplified processing strategies for the creation of 3D in vitro models of the airway tissues. While the initial focus of this research has been the lung, these materials and devices could potentially be used for organ-on-chip systems mimicking a variety of tissues. Some key aspects of this technology that we are researching are:

- The development of novel hydrogel-based materials to enable encapsulation of cells in 3D to better mimic the natural tissue organisation, either for culture in standard static conditions or for incorporation into the organ-on-chip devices: We are exploring hydrogels based on both naturally derived and synthetic materials, crosslinking using different mechanisms including photo-initiated free radical polymerization of hydrogel precursors as well as chemical crosslinking with naturally derived molecules such as genipin [1]. As an example, we have successfully encapsulated and grown human lung



(A) Human lung fibroblasts encapsulated in 3D in a gelatin-based hydrogel and cultured for 14 days; (B) human alveolar epithelial cells cultured for 72 hours on the electrospun membranes; (C) image of a PDMS microfluidic chip containing an electrospun membrane to create two channels in the device.

fibroblasts in 3D within a gelatin-based hydrogel to mimic the stromal tissue in the lung (Figure 1A).

- The use of electrospinning to produce membranes for incorporation in the microfluidic devices: We have manufactured membranes with pore sizes on the order of 1 micron that can also be used to support the culture of epithelial and endothelial cells in the airway-on-chip devices as well as in static culture (Figure 1B). These membranes are straightforward to prepare, and the physical properties of the membrane (thickness, pore size, tensile strength, etc.) can be tuned by varying the composition as well as the processing parameters.

- The implementation of additive manufacturing technologies for the creation of tailorable devices at low cost and with simplified processing steps: In the beginning, the fabrication of organ-on-chip devices used lithography techniques and silicon wafers to achieve the high-resolution features needed. However, advances in 3D printing techniques have been occurring at a rapid pace, which would reduce the cost and complexity of preparing organ-on-chip devices. We have developed processing workflows for the fabrication of devices out of polydimethylsiloxane (PDMS) using low-cost 3D printers and photo-polymerizable resins to create the molds. The final PDMS devices can further incorporate the electrospun membranes (Figure 1C) and be attached to microfluidic systems to enable perfusion. We are also interested more broadly in the development of biocompatible and photo-curable resins for use with stereolithography-based 3D printing techniques [2].

For more information, please contact
Dr. Jennifer Patterson at jennifer.patterson@imdea.org

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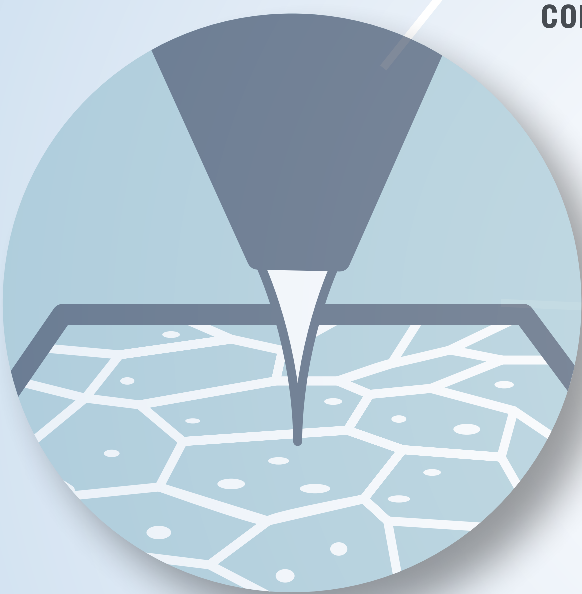
This work is funded through the project "MAMAP - Materials and models against pandemics" (REACT-EU resources of the Madrid Operational Program 2014-2020, in the action line of R+D+i projects in response to COVID-19). Project funded by the Community of Madrid and by the European Regional Development Fund of the European Union "A way to make Europe". Financed as part of the Union's response to the COVID-19 pandemic, through the agreement signed between the Community of Madrid (Regional Ministry of Education, Universities, Science, and Spokesperson) and the IMDEA Materials Foundation for the direct granting of a grant of 1.937.000.00 euros to fund research activities on SARS-COV 2 and the COVID-19 disease funded with REACT-EU resources from the European Regional Development Fun.

programme Advanced Manufacturing

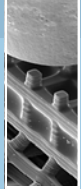
Structural composites

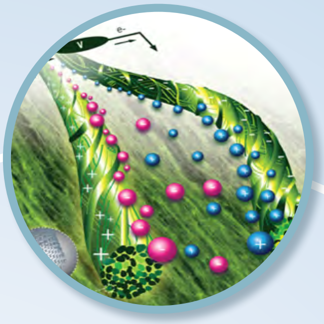


Goal and vision

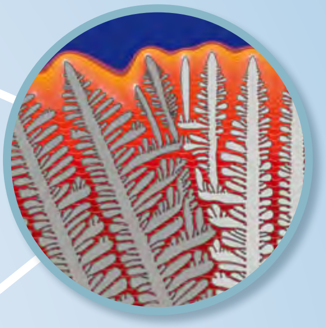
The programme on Advanced Manufacturing is highly interdisciplinary in nature spanning the fields of alloys, biomaterials, polymers, composites, energy materials, and involving both experimental and computational efforts. The objective of this programme is to improve quality, productivity, cost efficiency and sustainability in current manufacturing paradigms, as well as conceive and develop novel hybrid manufacturing techniques to enable the commercial realisation of emerging products in the aerospace, biomedical, energy, automotive and other industrial sectors.

Effective unit-process innovation and development derives from an understanding of the physical and chemical phenomena influencing manufacturing processes. Therefore, a key part of this programme involves the creation and development of models based on Artificial Intelligence (AI) to predict the optimum manufacturing routes and quality of the manufactured products, as well as the modelling and understanding of tool-material interactions. This fundamental knowledge is supplemented by state-of-the-art characterisation techniques needed to monitor the quality of manufactured products including their (micro)structure and mechanical and functional properties.





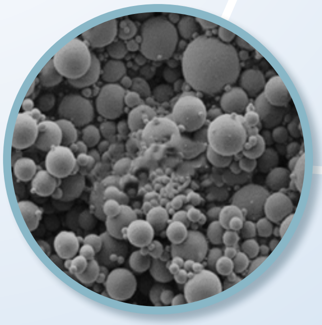
Multifuncional
Nanocomposites

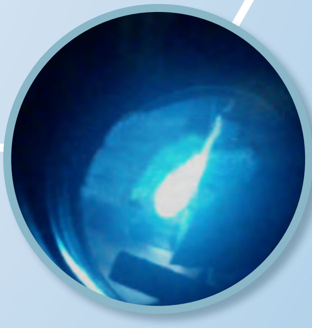


Physical Simulation

Modelling and
Simulation of
Materials Processing

Sustainable
Metallurgy





Sustainable
Powder
Metallurgy

Solidification
Processing & Engineering

Main research lines

Industry 4.0

- Virtual testing of structural composites. Analysis of the effect of manufacturing defects on structural performance.
- Virtual processing of structural composites including hot-forming and out-of-autoclave (injection, infusion, compression moulding). Surrogate and reduced order models for manufacturing based on multiphysics simulations.
- AI techniques applied to manufacturing. Digital twins for manufacturing processes. Smart detection of defects by sensors including the active control of manufacturing systems.
- Structural health monitoring (SHM) with carbon nanotuve yarns integrated sensors. Automated damage detection models based on AI.
- AI-guided materials design and chemical process.
- Electric current-assisted curing for bondings and repairs.
- Multifunctional composites for structural and energy storage applications.

Bulk nanostructured materials

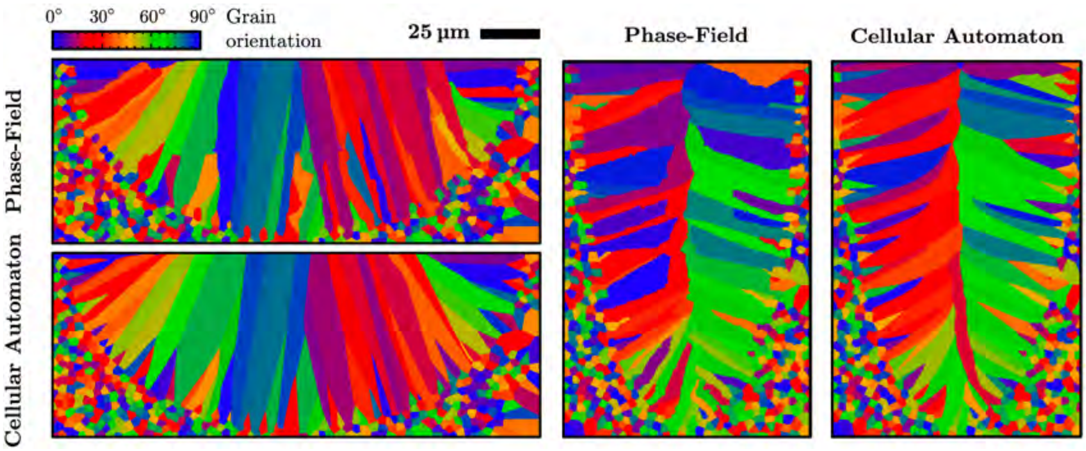
- Gas-phase assembly of continuous fabrics and fibres of carbon nanotubes and inorganic nanowires (Si, SiC).
- Integration of these nanostructured fabrics into electrochemical devices and composite materials.

Liquid and solid-state processing

- Rapid alloy prototyping and manufacturing of bulk alloy libraries for the fast assessment of properties.
- Optimisation of casting processes.
- Development of novel thermo-mechanical processes and powder metallurgy routes via mechanical alloying and gas atomisation in non-oxidation conditions.
- Consolidation by field-assisted sintering and conventional press and sintering.

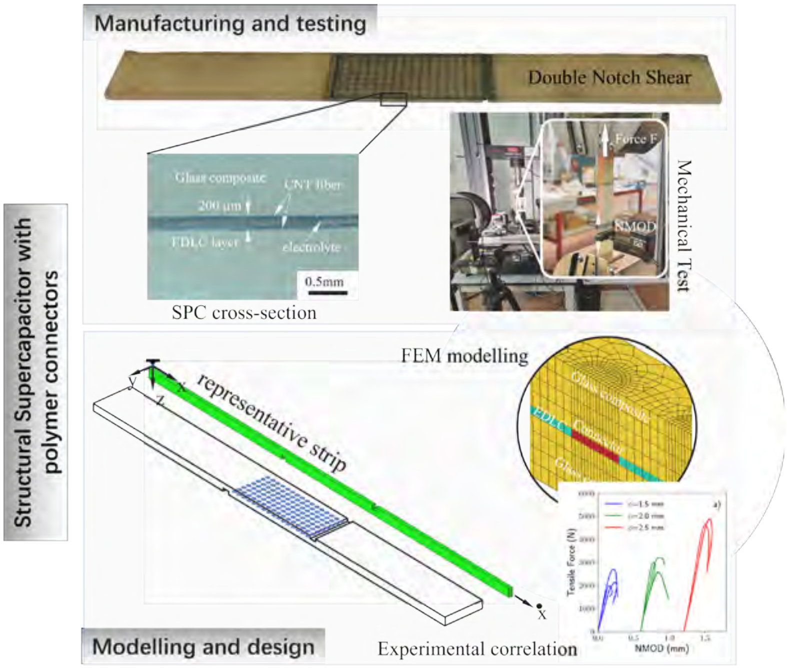
3D printing

- Metallic materials, including powder design, fabrication and characterisation.
- Composites, polymers, recycled fibers and hybrids.
- PLA composite materials reinforced with Mg, Zn or CaPs nanoparticles and continuous metallic wires.
- Development of functional thermoplastic filaments (flame retardant, thermal conductive, biodegradable, reinforced, electrically conductive, etc) for 3D printing.
- Data-driven design of 3D printed metamaterials.
- Custom made implants using new biocompatible alloys.

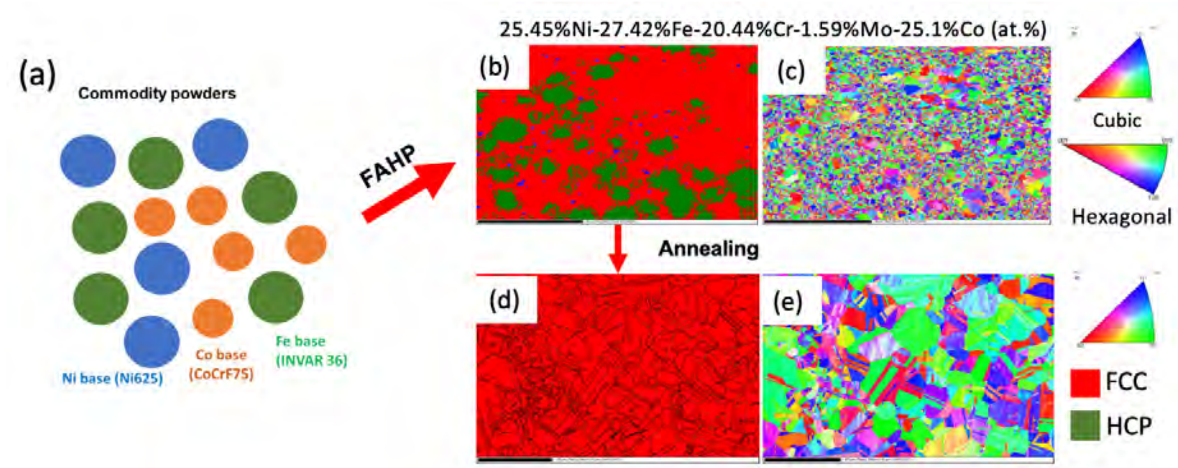


Grain orientation maps in cross-sections of laser-melted Ni alloy with different melt pool aspect ratio simulated using phase-field or cellular automaton methods.

- Stereolithography, including resin synthesis and characterization.
- Extrusion-based 3D printing of biomaterials and bioprinting.
- Predictive simulation.
- In-situ monitoring.



Assessment of stress transfer in laminated structural power composites produced with mechanically-connected electric double-layer capacitors.



A graphical abstract showing the process of developing the high entropy alloy starting from (a) a mix of commodity powders, (b) phase map and (c) Inverse pole figure (IPF-Z) map of the alloy obtained by EBSD after sintering by Field assisted hot pressing, (d) phase map and (e) IPF map of the alloy after annealing at 1200ºC for 24 hours.

Projects in focus

QPINOX / Development of New Martensitic Stainless Steels for Automotive Lightweight Structural Applications

Funding: European Commission/ Research Fund for Coal and Steel
Partners: IMDEA Materials Institute, TU Delft, CSM-RINA (Coordinator), ACERINOX SPA
Project period: 2019 - 2022
Principal Investigators: Dr. I. Sabirov and Prof. J.M. Molina-Aldareguia

In recent decades, there has been significant material development in the field of automotive applications, particularly in advanced high-strength steels (AHSS). This progress has been driven by lighter vehicles generating lower CO_2 emissions, coupled with passenger safety. Most recently, AHSS produced by quenching and partitioning (Q&P) heat treatment or by hot stamping, have pushed further the boundaries in terms of realisable strength and ductility combinations. To reach higher limits, AHSS have emerged as an appealing option for lightweight automotive applications.

Nevertheless, the development of AHSS faces certain challenges. These include the high cost of alloying elements, such as nickel in austenitic stainless steels, or the low ductility and formability of standard martensitic stainless steels. One potential solution to these issues is to create a new class of martensitic stainless steels by combining tailored chemical compositions and innovative heat treatments, such as Q&P. By incorporating retained austenite into the microstructure, it becomes possible to develop low-cost, high-strength, and ductile martensitic stainless steels suitable for automotive applications.

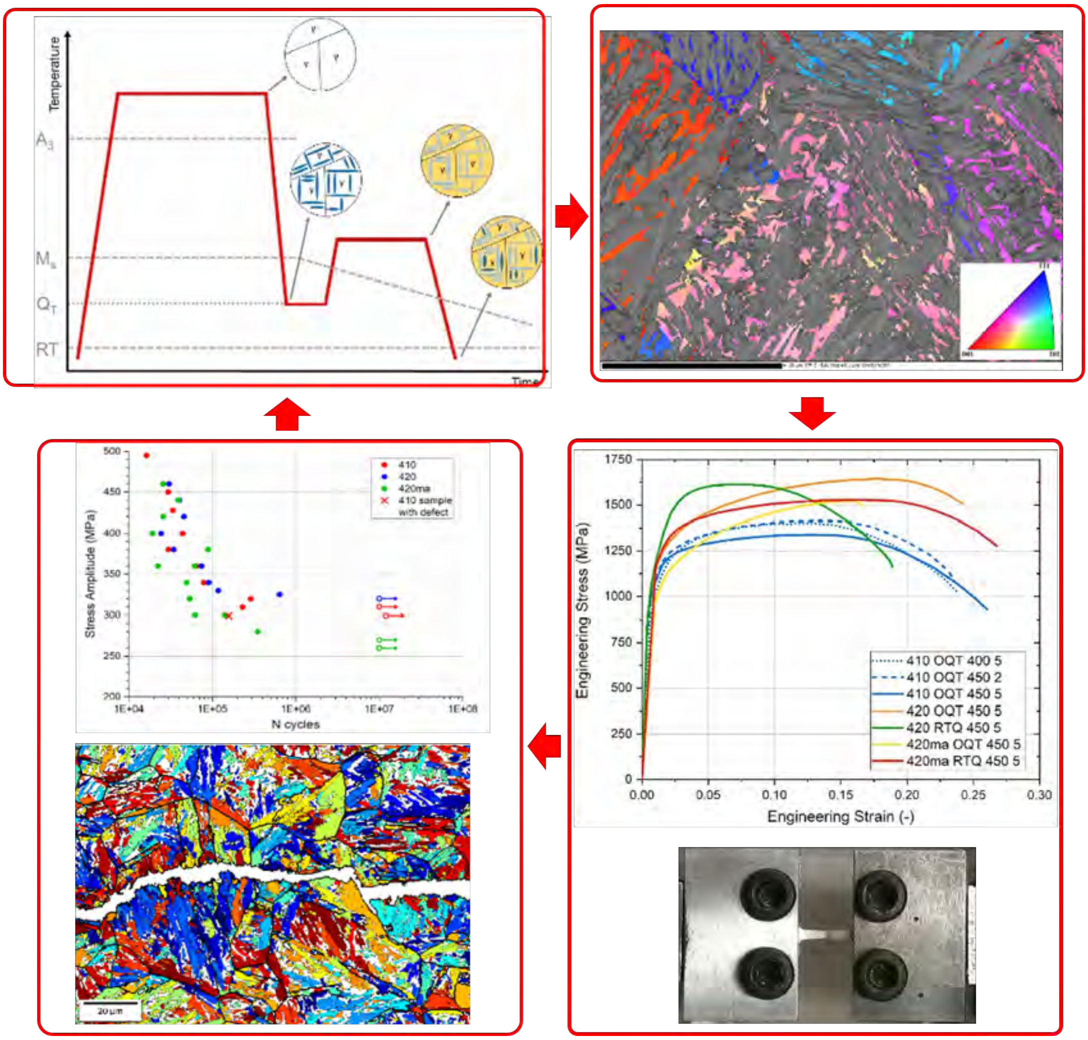
The QPINOX project aimed to address these challenges by generating a new class of affordable martensitic stainless steels, using the concepts of alloy design and Q&P treatment. The optimum hardenability of these martensitic stainless steels allows retained austenite to form at room temperature, also for low cooling rates. This greatly simplifies the heat treatment and facilitates industrial implementation. The main results of the QPINOX project include:

- Processing routes involving Q&P treatment were developed to manufacture 3 grades of martensitic stainless steel, which contain high fractions of retained austenite. Tensile strengths achieved ranged from 1300 to 1500 MP, with total elongation values ranged from 11.9 to 13.3%. A comparison with different AHSS showed that the developed steels possess similar or better combinations of strength and elongation (Fig. 1).

- The application-related properties, such as high cycle fatigue resistance, wear resistance, formability, weldability and corrosion resistance of these materials were explored (Fig. 1). The effect of the microstructure on their performance was understood, and the critical microstructural parameters were determined. It was demonstrated that the better application related properties can be achieved in Q&P stainless steels compared to those of their conventional counterparts.

- The manufacturing of the developed steels as annealed sheets was shown to be feasible with existing equipment.

- A production route for a new class of stainless structural automotive components has been established. Two options were proposed for component forming. For more simple shapes, the user performs the QP treatment on cut blanks followed by cold forming of the component shape. For more complex geometries it is proposed that the cut blanks are first cold formed to produce the component shape. The Q&P treatment is then performed on the component itself as a post-forming heat treatment.



Concept of QPINOX project. Top: Q&P treatment led to microstructure with high fraction of retained austenite. Bottom: Tensile mechanical properties are studied with respect to the microstructure. Selected conditions are subjected to high cycle fatigue testing. The outcomes of mechanical characterisation are used for tuning Q&P treatment parameters.

Overall, the QPINOX project successfully developed a new class of martensitic stainless steels for automotive applications, addressing challenges related to strength, ductility, and cost. The project also demonstrated the feasibility of manufacturing and utilising these materials in the automotive industry.

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Publications

A. Sierra-Soraluce, G. Li, M. J. Santofimia, J. M. Molina-Aldareguia, A. Smith, M. Muratori and I. Sabirov. *Effect of microstructure on tensile properties of quenched and partitioned martensitic stainless steels*, Materials Science and Engineering A. 864 (2023) 144540. https://doi.org/10.1016/j.msea.2022.144540

Research highlights

Additive manufacturing of amorphous soft magnetic materials

IMDEA Materials is participating in the EU Pathfinder OPEN project AM2SOFTMAG, which aims to develop the next generation of soft magenetic materials (SMM) for more efficient and cleaner devices by applying additive manufacturing (AM). Preliminary studies of the EU consortium resulted in the partially amorphous rotor shown in Fig. 1. New alloy compositions that are suitable for laser powder bed fusion processing need now to be developed ad hoc during the project in order to achieve 100% amorphicity of the SMM components.

Amorphous alloys are considered as the perfect match for AM because of the absence of solidification shrinkage that minimises cracking during the AM-production and because they exhibit superior soft-magnetic properties in combination to extraordinary mechanical hardness and strength. In contrast to traditional SMM, they are endowed with a unique combination of high resistivity, near zero coercivity, and high magnetic permeability values, and they can thus operate with extremely low electric power losses.

The technology developed within the AM2SOFTMAG project could substantially impact the propulsion of all-electric vehicles, and thus contribute to eliminate the highly polluting vehicle combustion engine altogether. The AM2SOFTMAG technology can be readily extended to build the next generation of all-electric trains, buses, trucks, as well as aircraft, thus allowing a radical reduction in global fuel consumption and of noise and pollution in metropoles over the next 10 to 15 years. The technology may also have a tremendously positive effect on the design of small electric motors for the quickly growing market of electrically motorised consumer goods, allowing for higher efficiency and silent operation with market entry shortly after project completion.

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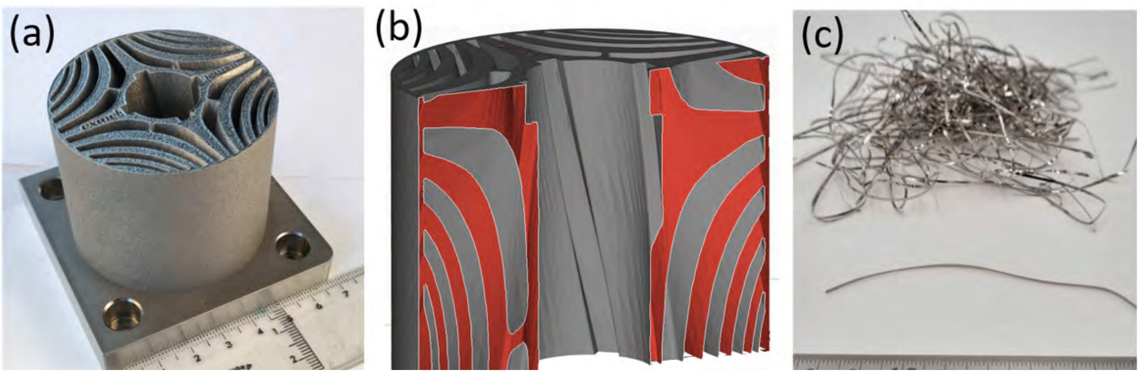

(a, b) AM processed rotor (EXMET) versus (c) as-spun ribbons.
Ref.: https://doi.org/10.1016/j.matdes.2022.110483

Advanced Carbon Nanotube Sensors for Structural Health Monitoring

Structural health monitoring (SHM) is progressively gaining importance in the aerospace and civil engineering sectors because of the need to detect early material damages that can prevent catastrophic failures. Structural carbon laminates are nowadays commonly used in these sectors due to their superior stiffness/strength-to-weight ratio. However, they are particularly challenging to SHM because of the complex anisotropic structure and diversity of the existing failure mechanisms ranging from matrix cracking, fibre fracture to ply delamination. Advanced sensors such as fibre optic sensors demonstrated excellent potential for SHM of composite laminates, although they are still too invasive and complex to integrate into the manufacturing process chain. IMDEA Materials is working in the H2020 DOMMINIO consortium together with AIMEN to develop a new generation of low-intrusive piezoelectric carbon nanotube fibre sensors that can be integrated into the structural laminate during the manufacturing process. Apart of their easy integration in the manufacturing chain, their weight makes them ideal candidates to reduce sensor wiring weight in aerospace applications.

The first step of the process starts with manufacturing a printable filament in which the carbon nanotube sensor is embedded in a polymeric material. The filament can be printed over the laminate surface during the lay-up operations, a process fully compatible with the standard laying techniques such as fibre placement (AFP) or manual lay-up. After laminate consolidation with the application of the corresponding thermal-pressure cycle, the sensor is fully embedded inside the laminate, providing the possibility of electrical interrogation. The change of its electric resistance can be endorsed to the total macroscopic strain acting on the embedding structural laminate. After mechanical interpretation, these sensors provide real-time data that can be used using artificial intelligence digital twins to infer laminate health, allowing for proactive maintenance and reducing the risk of catastrophic failure.

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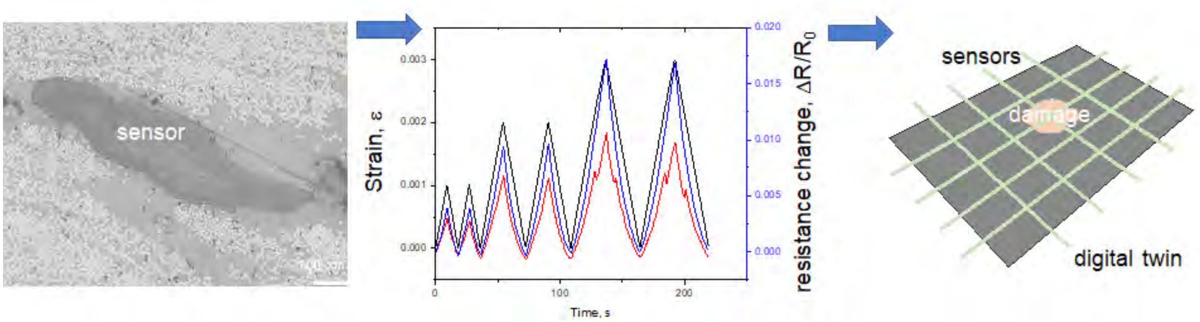
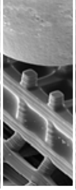


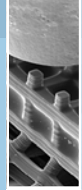
a) Cross section of an embedded continuous carbon nanotube (cCNTs) filament into a CF/thermoplastic polymer composite, b) Change of electrical resistance (blue and red) of two cCNTs filaments embedded in a coupon during the tensile testing in 6 load/unload cycles, c) Schematic of composite panel instrumented with a grid of embedded cCNTs filaments to detect damage in the panel and update this information to a digital twin of the component.

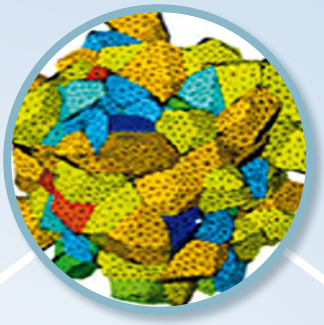


programme
Integrated Computational Materials Engineering

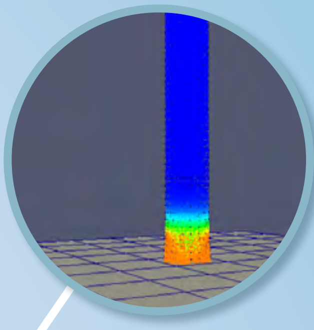
Goal and vision

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 optimised before they are actually manufactured in the laboratory. The focus of the programme is on materials engineering, i.e. understanding how the microstructure of materials develops during processing (virtual processing), the relationship between microstructure and properties (virtual testing) and how to optimise materials for a given application (virtual design). Moreover, experiments are also an integral part of the research programme for the calibration and validation of the models at different length and time scales. The expertise of the researchers in the programme covers a wide range of simulation techniques at different scales (electronic, atomistic, mesoscopic and continuum) and is supported by a high-performance computer cluster.

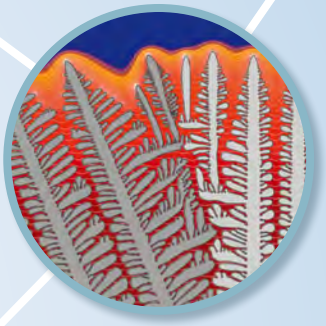




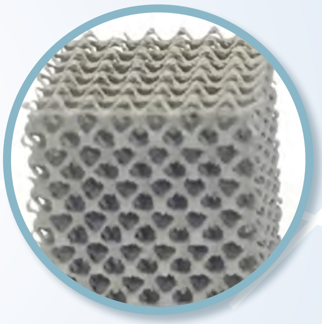
Multiscale Materials Modelling



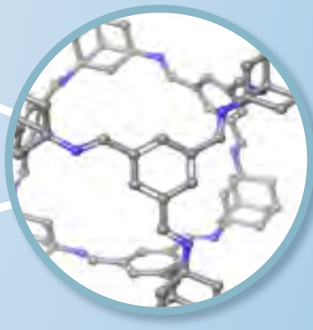
Computational Solid Mechanics



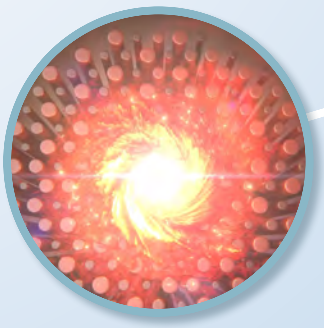
Modelling and Simulation of Materials Processing



Bio/Chemo/Mechanics of Materials



Computational and Data-Driven Materials Discovery



Acoustic and Mechanical Metamaterials

Main research lines

Virtual materials design, including virtual processing and virtual testing

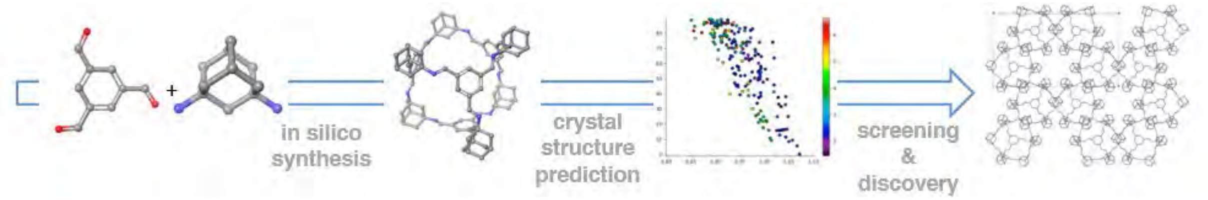
- Virtual material discovery for functional applications using DFT, cluster expansion and atomistic approaches combined with AI.
- Virtual processing: Integration of modelling tools (atomistic, computational thermodynamics and kinetics, phase-field) to simulate the microstructural development of materials during processing.
- Virtual testing of metallic alloys: Development of microstructural-based constitutive models to predict the mechanical behaviour of single crystals. Simulation of the mechanical response of polycrystalline metals by means of FFT and FEM based homogenisation.
- Virtual testing of composites: Implementation of the constitutive models in finite element codes to simulate the mechanical behaviour of structural components.
- Smart manufacturing: multiphysics models of autoclave and out-of-autoclave curing of composite materials accounting for porosity evolution during the process. Simulation-based smart manufacturing processes. Sensoring and process control.
- These approaches are applied to several materials, in particular
  - Metallic alloys for engineering and biological applications
  - Multifunctional composite materials and structures.
  - Materials for catalysis.

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.
- Finite Element solvers for multiphysics problems.
- Fast Fourier based solvers for multiphysics problems.

Multiscale materials modelling

- Bottom-up approaches (scale bridging).
- Development of modular multi-scale tools.
- High throughput screening integration.
- Concurrent models.
- Mean-field homogenisation
- Computational homogenisation including FEM and Fast Fourier Transform –FFT–based solvers



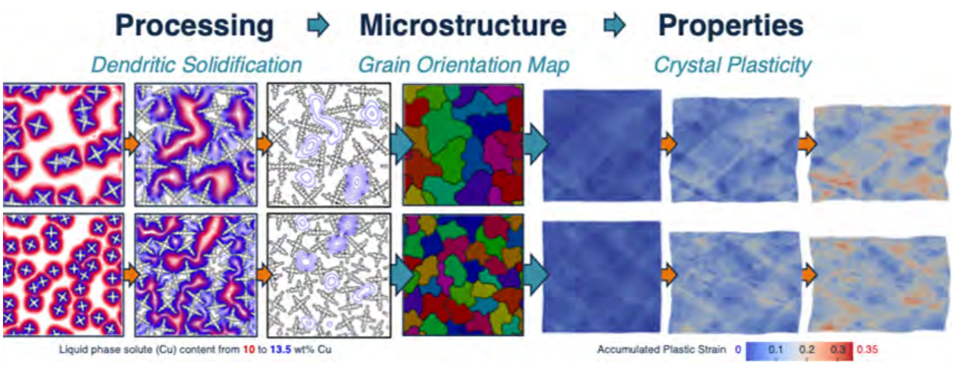
Computational, data-driven materials discovery

Modelling and simulation strategies for different applications

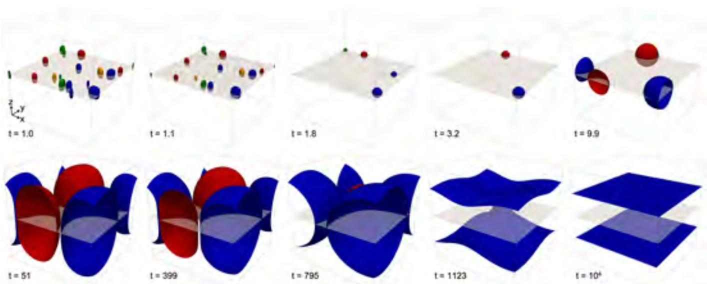
- Material informatics for analysis of large material datasets.
- Modelling and simulation of H_2 embrittlement in metallic tanks and pipes.
- Study of H_2 diffusion mechanisms in metals.
- Discovery of new catalysts for H_2 production and fuel cells.
- Discovery of new catalysts for CO_2 reduction reaction.
- Modelling and simulation of multiscale transport phenomena (application to advanced materials for batteries).
- Virtual design and testing of mechanical metamaterials and architected metamaterials
- Simulation of the additive manufacturing process in metals including macroscopic simulation of the thermomechanical process by multiphysics finite element models, microstructure evolution through phase field and prediction of mechanical response using polycrystalline homogenization.
- Modelling and simulation of elastic waves and sound propagation in complex additive manufactured media
- Exploring new physical phenomena in the wave-based and elastostatic context

Computational and data-driven materials discovery

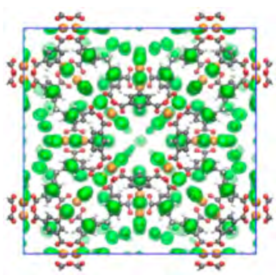
- Discovery of porous materials for energy applications (CO_2 capture, methane storage).
- Design of ionic liquids.
- Materials discovery: structures with high H_2 working capacity and H_2 adsorption-desorption performance.
- Design of Metal-Organic Frameworks (MOFs) for separation of gases for anaesthesia (Xe/Kr).



Linking processing, microstructure, and properties by coupling multiscale models – here, dendritic needle network solidification model with crystal plasticity model



Phase-field simulation of microstructure evolution accelerated by semi-implicit FFT-based solver
[Boccardo et al., Computational Materials Science 228 (2023) 112313]



Predicted distribution of Xe atoms in MOF

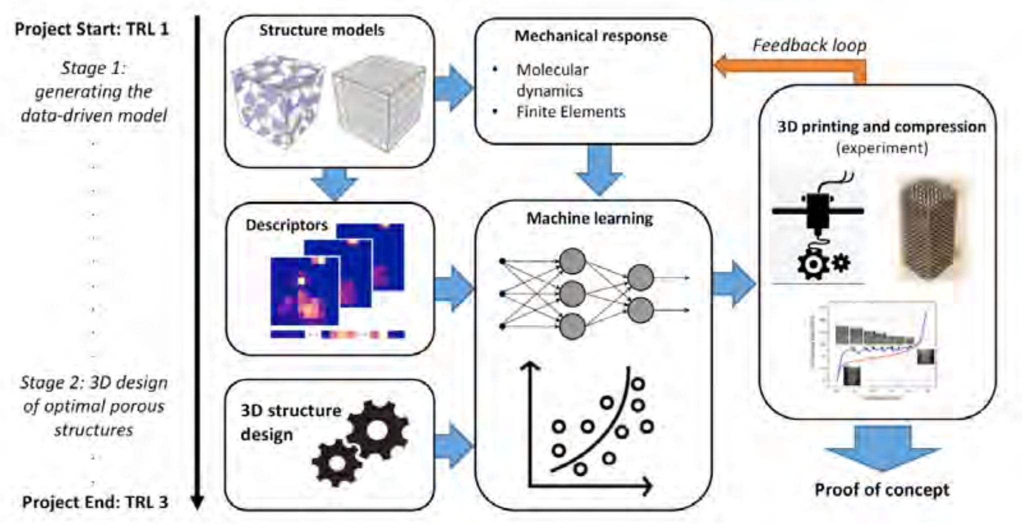
Projects in focus

PORMETALOMICS / Porous Metal Genomics for Tailoring Mechanical Properties of Light-weight 3D-Printed Architectures

Funding Institution/Programme: M-era.Net
Partners: IMDEA Materials Institute (coordinator), Technion – Israel Institute of Technology and the Institute of Mathematics of the Polish Academy of Sciences (IMPAN).
Project period: 2022-2025
Principal Investigators: Dr. M. Haranczyk, Dr. M.T. Pérez-Prado and Dr. I. Romero

Porous metals, with pore diameters from nano to millimeters, are increasingly important in technology. Their high surface-to-volume ratio together with optimisable mechanical properties makes them promising candidates in various emerging applications such as metallic scaffolds for load-bearing bones, lightweight structures for transport technologies, electrodes for electrochemical energy storage devices and more. Additionally, 3D printing opens new horizons in additively manufactured complex porous architectures with desired properties. However, the enormous variety of possible morphologies makes it non-trivial to optimise the structure to tailor its mechanical properties. In order to fully harness the opportunities created by porous structures and to successfully incorporate them in next-generation devices, PORMETALOMICS aims to build (a) fundamental understanding of the relation between the structure's morphology and the mechanical properties across the length-scales; (b) quantitative and exploitable structure-properties relationships, and (c) implement machine learning-based design in the vast morphological configuration space. These new capabilities will be incorporated into state-of-the-art 3D printing, enabling the creation of tailor-designed structures with desired mechanical properties.

In order to achieve the aims of this project, we bring together expertise in applied mathematics, material informatics, atomistic and continuum simulations and 3D printing capabilities. We are developing a cutting-edge methodology to characterise the morphology of porous structures. The resulting geometrical and topological



Workflow to be implemented within PORMETALOMICS descriptors will be used to characterise a large number of morphologies as well as to enumerate new structures with statistical importance, e.g. with unique topologies and/or geometries. Material modelling tools applied to the same data will give their mechanical response to load, paving the way to direct relation between invariants and mechanical properties. The latter, captured within machine learning models, will be employed to assess the mechanical property of various prototype structures of new morphologies via implementation of hierarchical screening, genetic algorithms or other machine learning techniques.

Finally, an experimental 3D-printing effort is being tightly integrated with the modelling part of the project with the goal of experimental verification of methodology, hyperparameter tuning, and execution and characterisation of the identified important (e.g. best-performing) candidate structures. Specifically, the project's main outcome will be prototypes of new lightweight metal structures with desired mechanical properties and high porosity.

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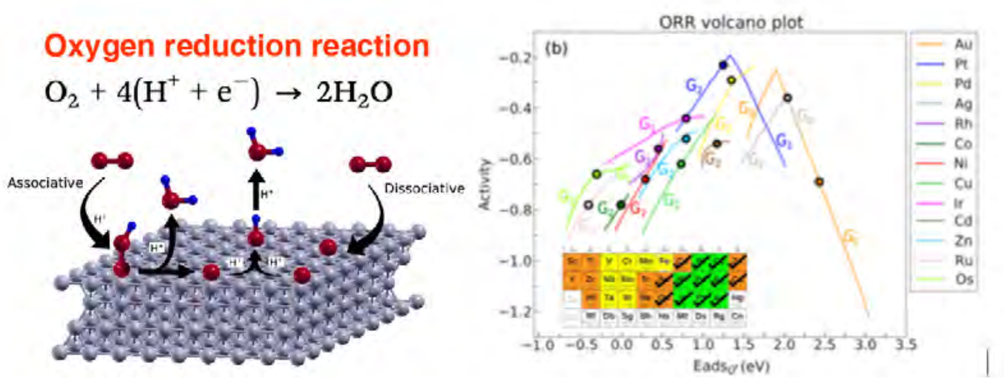
Research highlights

High-throughput discovery of new catalysts for the hydrogen economy

The 7th sustainable development goal of the United Nations is to ensure access to affordable, reliable, sustainable and modern energy for all while the 13th goal is to take urgent action to combat climate change. Both objectives are closely linked to the use of clean and renewable energy sources for addressing the world's rising energy needs while limiting environmental effects. However, further expansion of renewable energies (currently 28% of world's electricity) is limited because power provided by solar and wind energy (as opposed to coal, natural gas and nuclear) is intermittent and has to be associated with large energy storage capabilities. Hydrogen energy storage offers a unique combination of scalability, long-term storage and portability, leading to the so-called hydrogen economy. In this model, renewable energy sources are used to split water into hydrogen and oxygen. The hydrogen is stored for later use in fuel cells or gas-fired turbines to generate electricity without emission of pollutants.

However, the expansion of the hydrogen economy is limited by the sluggish kinetics of the hydrogen evolution reaction (HER) for production of hydrogen from water and of the oxygen reduction reaction (ORR) for the generation



(a) Schematic of oxygen reduction reaction (ORR) on a surface catalysts. (b) Volcano plot of the catalytic activity for the ORR as a function of the applied strain 13 transition metals showing the potential of this strategy to improve the catalytic performance (C. Martínez-Alonso, J. M. Guevara-Vela, J. LLorca, Physical Chemistry Chemical Physics, 24, 4832–4842, 2022)

of energy from hydrogen. This limitation can only be overcome by the use of Pt as catalyst and, thus, the search for efficient and affordable catalysts for the HER and ORR is a critical priority to ensure the success of the hydrogen economy. Within this context, the project CATBYESE funded by the Spanish Ministry of Science and innovation through the call for Green and Digital Transition projects is aimed at developing a high-throughput methodology based on the application of first principles calculations and artificial intelligence to discover new catalysts (or improve the performance and / or selectivity of existing catalysts) by modifying the electronic structure through the application of elastic deformations (see figure). The new catalysts candidates will be manufactured by magnetron sputtering in the form of thin films (thickness <50 nm) on suitable substrates. In these films, intrinsic elastic deformations will be introduced during the deposition process on substrates with different thermal expansion coefficients or by means of heat treatments on thin films deposited in shape-memory alloys while extrinsic elastic deformations will be applied by deforming the substrate/film with mechanical devices. Finally, the electro-catalytic activity and durability of thin films for HER and ORR reactions will be determined via voltammetries and impedance spectroscopy in an electrochemical cell capable of being coupled to mechanical testing units. To do this, mechano-electrochemical cells will be designed and manufactured to carry out electrochemical experiments in situ while the coatings are subjected to either intrinsic and/or extrinsic elastic deformations. If successful, the strategies and tools developed in this project can be applied latter to many other catalytic processes of large industrial importance.

For more information, please contact
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[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.

Bayesian calibration of material models

The sciences do not try to explain, they hardly even try to interpret, they mainly make models.

John von Neumann (1903-1957)

Everywhere in science, we find models. In particular, in Materials Science we build models to understand and predict the behaviour of materials at all scales, under very different external conditions (temperature, stress, deformation, radiation, humidity, etc.) Maybe with the exception of Schrödinger's equation, everywhere else material models depend on parameters whose precise value is unknown. The accuracy and robustness of these models in thus contingent on the value selected for these parameters and often experimental campaigns are designed to pinpoint their value.

In the simplest models, parameters are given a fixed numerical value. This value might be the one leading to model predictions that have the smallest mean squared error relative to the available experimental data. But material scientists know better: no experiment gives always the same response and mean values are always accompanied by *error bars* that, even if roughly, account for the variability of the tests. Hence, if experiments are in a way *stochastic*, parameters should be too. This has led to considerable interest in more sophisticated calibration techniques, ones that can identify the complete *probability distribution* of a model parameter, not only its point value.

IMDEA Materials has participated in project HUC of the Clean Sky 2 programme, together with CEIT, Aubert & Duval, INSTM, UPV, and ITP, who led the project. In this project, the Computational Solid Mechanics group led by Prof. Ignacio Romero has been in charge of the calibration of complex material models, of the type typically employed to simulate the mechanical response of metals under high strain rates, high stresses, and high temperatures. The main goal of the project was the design and analysis of a turbine case for a new jet engine developed by ITP. Such a part should be tested in the most stringent conditions, including the impact of detached turbine blades, and numerical simulations become indispensable to explore potential failures. As advanced, the models for the material behaviour in these situations had to be calibrated before performing any simulation.

At IMDEA Materials we have developed a methodology for the *Bayesian calibration* of computer models and applied it to the thermomechanical response of Astroloy, the material chosen for the casing. As in any Bayesian model, the fundamental idea has been to update prior (and very uncertain) knowledge about the model parameters for this material, together with non-parametric machine learning models and obtain optimal *posterior* probability distributions for the material parameters. This had to be done for over twenty scalar parameters that are employed to represent the response of the material under extreme conditions and its changes as the material ages. To perform the calibration, synthetic data obtained from simulations had to be combined with experimental data points obtained by the Physical Simulation group at IMDEA Materials, led by Dr. Ilchat Sabirov and the Materials Science department at the ETSICCP of the Technical University of Madrid. This hybrid source of virtual and physical tests can be used to build a *surrogate model* for the material response than can be queried thousands of times to find the optimal values of the parameters. See Fig. 1 for an example of a physical and a digital test of an impact experiment, both employed to calibrate the model.

As shown in Fig. 1, the outcome of the Bayesian analysis is a complete probability distribution of each of the model parameters for the material of interest (only two are shown). This characterisation is a proxy for the uncertainty of the model and was employed to determine which experimental campaigns needed to be extended, to reduce the uncertainty of the calibration. More advanced uncertainty quantification of the predictions could be obtained using Monte Carlo techniques, although they were not part of the objectives in HUC.

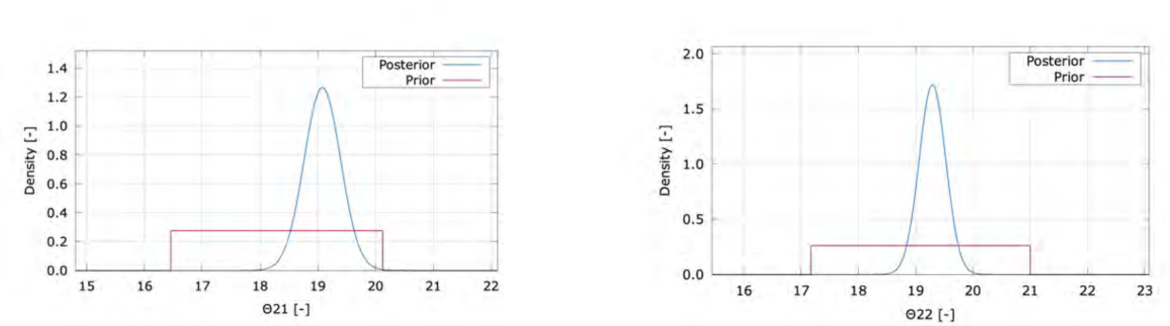

Fig. 1. Prior and posterior probability distributions of two calibration parameters.

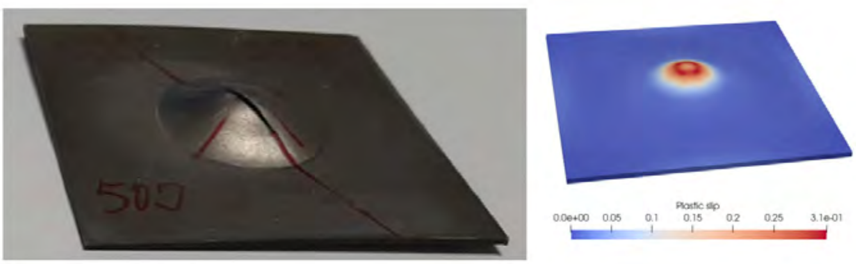

Fig. 2. Experiment and simulation of impact test.

To close, the calibration of computer models using Bayesian techniques is an extremely useful tool that goes well beyond the determination of optimal values for material models. It is linked with the formulation of more reliable models, ones that can not only predict physical behaviour but simultaneously ascertain their uncertainty in a rigorous fashion.

For more information, please contact:
Prof.Ignacio Romero at ignacio.romero@imdea.org

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[1] J.L. de Pablos, I. Sabirov, I. Romero. *A methodology for the calibration of complex material models: application to thermo-elasto-plastic materials for high-velocity impact simulations.* Archives of Computational Methods in Engineering. 30 (2023) 2859-2888. DOI: 10.1007/s11831-023-09888-y.

Numerical models for elastic wave propagation in heterogeneous media

It is very well known that the microstructure of a material has a strong influence in the propagation of elastic waves through it. In the case materials based on a repeating unit cell, the interaction of elastic waves with the microstructure might lead to the appearance of band gaps for which propagation of mechanical waves is hindered. This property is actively used to design such materials as wave guides or for cloaking applications. In the cases of random heterogeneous materials such as composites, polycrystals or porous materials, elastic waves also present dispersive. These effects are not reflected in the presence of bandgaps, but introduce a dependency of the wave propagation with the frequency that controls the penetration of waves in the material and/or modifies the wave velocity for wavelengths near the microscopic characteristic length (e.g. grain size or mean distance between second phases). In both cases, having tools able to predict the link between microstructure and wave propagation characteristics is fundamental to analyse the result of acoustic experiments or to design microstructures with special acoustic response.

Several analytical models are available which provide the acoustic response as function of some averaged features of the microstructure. However, in many cases the numerical resolution of the governing equations on a spatial domain considering explicitly a representation of the microstructure is necessary to obtain accurate results. The finite element (FE) method is the most common approach for solving these micromechanical problems. Nevertheless, numerical approaches based on the Fast Fourier Transform (FFT) algorithm, which have been extensively used in the last two decades for quasistatic micromechanical problems [1], present very high potential also for solving wave propagation within the microstructure. The main benefit of these approaches is their numerical performance compared to FE, which allows the use of very complex and detailed representation of the microstructure. Moreover, these methods are grid-based so meshing is not required allowing the direct use of images or tomographic data to create the models.

The Multiscale Materials Modeling group led by Prof. Javier Segurado have proposed, in collaboration with researchers from Los Alamos National Laboratory, some numerical approaches based on the FFT for solving elasto-dynamic problems in heterogeneous media. Regarding the frequency domain, a novel FFT-based method has been developed to obtain dispersion diagrams in periodic heterogeneous microstructures [2]. The method solves the Bloch-wave eigenvalue problem in a representative volume element (RVE) of the periodic microstructure, to obtain the set of frequencies at with a harmonic wave of a given length and propagation direction can propagate. This approach allows to obtain very efficiently bandgaps in composites or lattice metamaterials and can be used to study wave speed attenuation as function of frequency. As an example, Fig 1. one shows the result of applying this method to a porous material. In Fig 1a. the resulting dispersion diagram is represented, showing a frequency bandgap, together with one of the deformation modes. In Fig 2a. the method is applied to a random polycrystal providing the attenuation of the group velocity as function of wave length.

A second approach is proposed in [3] to simulate the propagation of elastic waves in time in heterogeneous domains which also relies on the use of the Fourier Transform to solve for every time step the distribution of microscopic fields in the microstructure. The method allows one to prescribe the displacement as a function of time in a subregion of the domain. Equations are efficiently integrated using an unconditionally stable beta-Newmark approach which allow the use of time steps much larger than the stable increments in typical explicit FE solvers. The accuracy of the method is similar or better than that of the implicit FE method and the numerical efficiency surpasses fast explicit FE approaches and can be orders of magnitude faster than implicit FE, allowing the use of much larger models. This method has been used to study propagation of a pulse on a polycrystalline bar (Fig 2a). The numerical resolution allows to reproduce the effect of scattering with grain boundaries. For long pulses, scatter is minimal, and wave behaves as in a monolithic media with homogeneized response (Fig 2b). On the contrary, for short pulses, scatter with grain boundary strongly affects pulse propagation (Fig 2c). The method can be used to simulate complex three-dimensional acoustic experiments, such as the RUS (Resonant Ultrasound Spectroscopy), in order to analyze the effect of microstructure in the experimental response.

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

References

[1] S. Lucarini, M. Upadyhay, J. Segurado. *FFT based approaches in micromechanics: fundamentals, methods and applications.* Modelling and Simulation in Materials Science and Engineering 30 023002, 2022.

[2] R. Sancho, V. Rey de Pedraza, P. Lafourcade, R.A. Lebensohn, J. Segurado. *An implicit FFT-based method for wave propagation in elastic hetergeneous media,* Computer Methods in Applied Mechanics and Engineering 404, 115772, 2023.

[3] J. Segurado, R. Lebensohn. *An FFT based approach for Bloch wave analysis: application to polycrystals.* Computational Mechanics 68 (5), 981-1001, 2001.

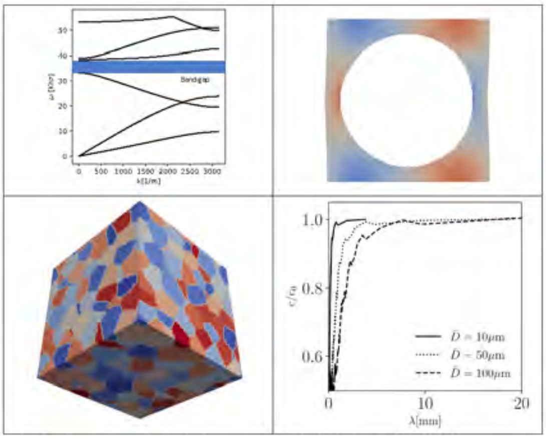


Fig. 1. (a) Left, dispersion diagram showing a band gap in a porous material with 50% of porosity. Right: RVE of the porous material showing one of the oscillation modes found (b) Left: RVE of a polycristal microstructure. Right: Results of group velocity (c/c0) attenuation with respect homogeneous metal in the polycristal as function of the wavelength for different grain sizes (D)

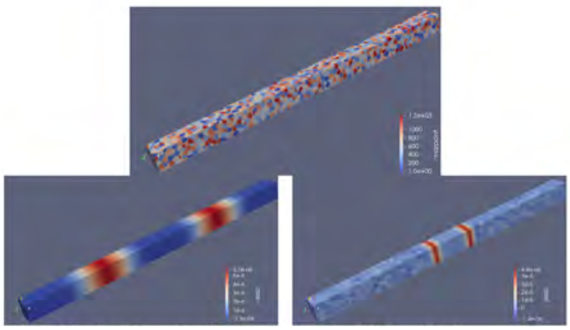


Fig. 2. (a) Metallic bar with explicit representation of the polycristalline microstructure. (b) Displacement due to the propagation of a long pulse. (c) Displacement due to the propagation of a short pulse showing the scatter with grain boundaries.

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 the microstructure of the material in focus, its evolution during either processing or service operation, and its influence in the relevant properties for the purpose it was designed. 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 distribution and evolution in advanced materials during processing and service using advanced characterisation techniques.


Sustainable Metallurgy
Multifunctional Nanocomposites
Nanomechanics y Micromechanics
Structural Composites
Bio/Chemo/Mechanics of Materials
Sustainable Powder Metallurgy
X-Ray Characterisation of Materials

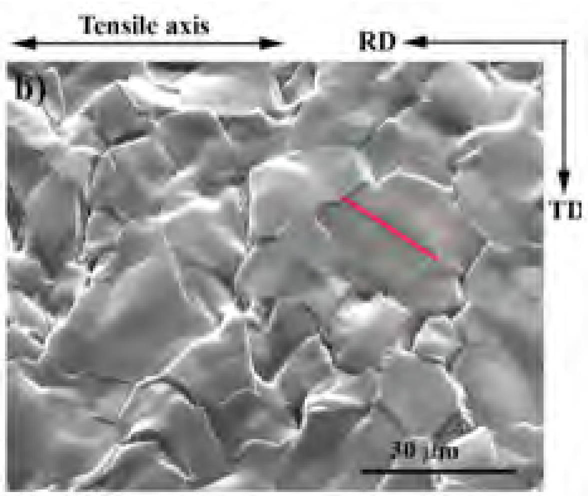
Main research lines

Advanced material characterisation, including microstructural, chemical and crystallographic information across several length scales and using different techniques

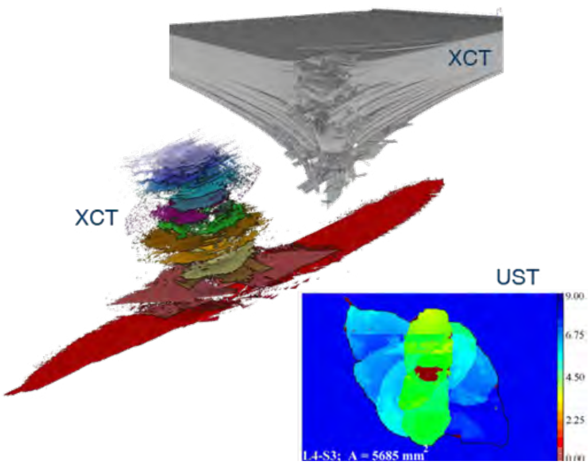
- Multiscale characterisation with optical and electron microscopy, X-rays, atom force microscopy, Raman spectroscopy, ultrasonic inspection. Some of the equipment we use for this are:
  - FIB-FEG-SEM, including 3D-EDS and 3D-EBSD. In-situ stages for thermomechanical testing
  - FEG-TEM including 3D-STEM and 3D-EDS with in situ stage for mechanical testing
  - X-Ray Tomograph (XCT) with in situ stage for thermomechanical testing, furnaces for thermal treatments and observation of chemical reactions, in situ composite curing, in situ composite infiltration
  - X-ray Diffractometer (XRD) equipped for residual stresses and texture determination, reflectometry analysis, Cu and Cr radiation, linear detector, in -situ furnace.
  - Raman micro-spectrometer 5x, 20x, 50x, 100x microscope objectives, 532 nm Nd:YAG laser (50W) and diffraction grating of 1800 l/mm, 100 nm resolution.
  - Small angle X-ray scattering and Wide angle X-ray scattering (SAXS/WAXS) for the study of crystallization in polymers, chemical composition or phase composition of a film, the texture of a film (preferred alignment of crystallites), the crystallite size and presence of film stress.
- Characterisation of broad range of materials, e.g. biomaterials, plastics, metal matrix composites, fibre reinforced composites, metals, nanomaterials, etc.
- Use of large facilities such as neutron or synchrotron radiation facilities for characterisation
- Development of new methodologies (e.g. hardware for in situ testing and software tools) for material characterisation and analysis, also applying artificial intelligence methods.
- Correlative studies of materials, i.e. combining insights from different techniques.

4D characterisation: in-situ multiscale characterisation of processes

- Thermo-mechanical testing across several length scales: tension, compression, fatigue, creep, etc. in the scanning electron microscope and X-ray tomograph.



Deformation of polycrystals observed in SEM

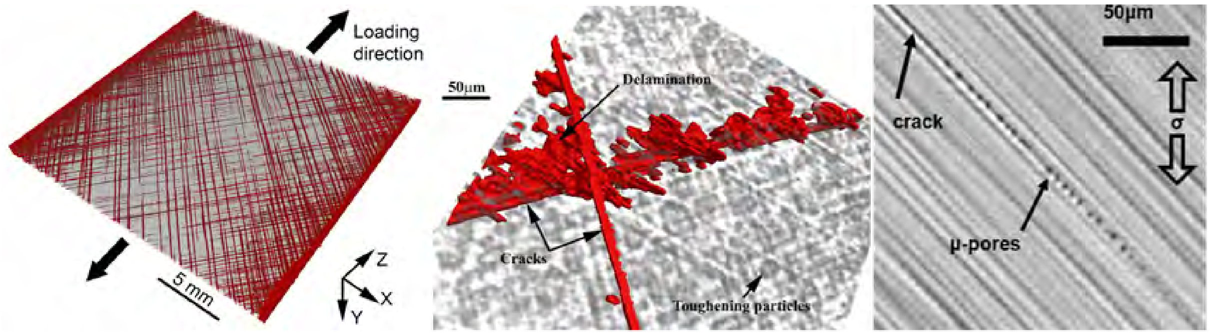


Automatic damage extraction of 3D volumes by XCT and AI correlative techniques

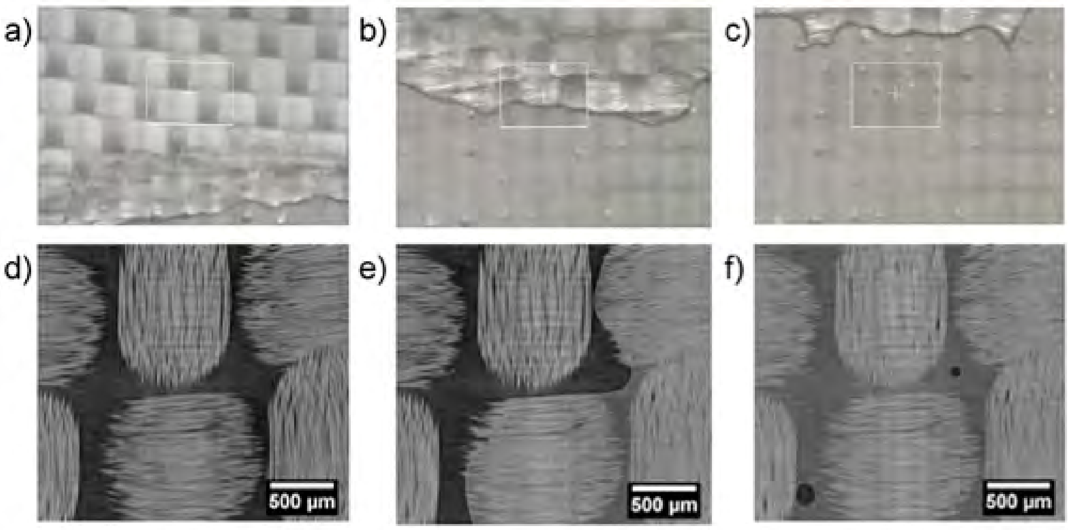
- Properties and deformation mechanisms of small volumes by nanomechanical testing in the scanning and transmission electron microscopes: properties of metallic phases, interfaces, nanoparticles, carbon-based nanomaterials (carbon nanotubes, graphene, etc).
- Elevated temperature nanomechanical testing.
- 4D characterisation of processes by X-ray tomography and X-ray diffraction: e.g. metallic alloy solidification, metallic alloy phase formation and chemical reactions, infiltration and resin flow in composites, composite curing, etc.

Cross-correlation between experiments and multiscale simulations (molecular dynamics, dislocation dynamics, crystal plasticity, finite elements, etc)

- Digital modelling from 3D structures.
- Integration of experimental statistical measurements into models.
- Experimental confirmation of modelling results.
- Experimental design based on models.



Multiscale & in-situ damage quantification of engineering materials



Resin Transfer Moulding (RTM) processing during XCT measurement

Projects in focus

TOPOMAG-3D / Microstructure-topology-mechanical properties relationships of 3D printed Mg-based scaffolds for biomedical applications

MINISTERIO DE CIENCIA E INNOVACIÓN
UNIÓN EUROPEA
FONDO EUROPEO DE DESARROLLO REGIONAL

Funding Institution/Programme: FEDER/Ministry of Science, Innovation and Universities - State Research Agency

Principal Investigators: Dr. Federico Sket

Traditional implants for bone replacement are made of titanium alloys, stainless steel or cobalt alloys. Since they are not biodegradable, these materials often require a second surgery to remove the implants, as they can cause infection and inflammation problems. These problems can be eliminated using bioabsorbable metals that can gradually degrade or corrode in vivo. This approach would allow a significant improvement in the quality of life of people. According to the market research report published by Facts and Factors, the global orthopaedic implants market was valued at $50.6 billion in 2019. Furthermore, this market is expected to generate about $73.5 billion by 2026, growing at a compound annual rate of around 5.48% between 2020 and 2026. It is a field of great importance, which seeks innovation and the best solutions.

Magnesium (Mg) has the best potential for bone implants due to its biocompatibility and osteopromotional properties that can stimulate new bone formation, such as severe rupture or resection due to tumours. On the one hand, the elastic modulus of Mg is similar to that of human bone, which prevents the implant from absorbing the mechanical load and limiting bone regeneration.

In addition, porous scaffolds provide better integration with human tissue and accelerate the growth of new tissue. On the other hand, it is necessary to control the rate of degradation when the material is in contact with body fluids since pure Mg tends to degrade too quickly, leading to excessively high hydrogen release rates that can be toxic in cellular environments. In this sense, the alloying of Mg with rare earth elements improves both mechanical strength and corrosion resistance.

To achieve optimal conditions for these materials, it is necessary to use novel processing techniques that allow the manufacturing of Mg scaffolds with complex geometry,

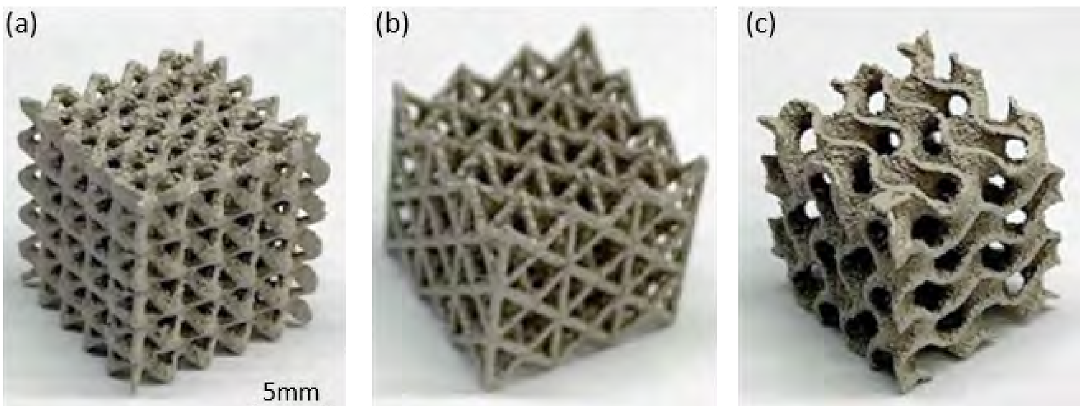


Fig. 1. Mg-based scaffolds with different topologies. a) BCC, b) FCC, c) Gyroid.

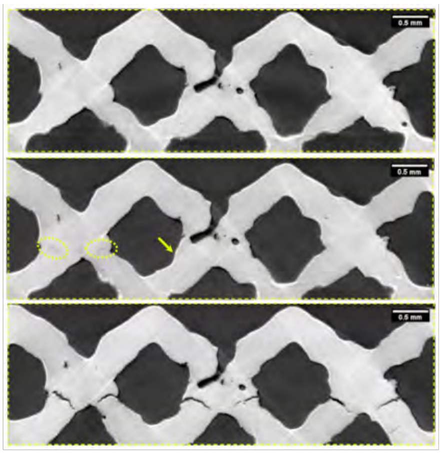


Fig. 2. Detail of loading sequence showing the fracture mechanisms on a BCC scaffold (unpublished data).

capable of withstanding mechanical loads, having an open porosity that allows vascularisation and bone regeneration, and being absorbed in the end of the process. This is intended to ensure that a second surgical intervention is not necessary for its removal.

Recently it has been possible to 3D print scaffolds of Mg alloyed with rare earth elements using selective laser melting (SLM) techniques, such as the one shown in Fig. 1. However, it is necessary to determine its mechanical properties and biodegradation processes to find those topologies that guarantee that the bone regeneration and bioabsorption processes are perfectly aligned and coupled.

This is the goal of TOPOMAG-3D project, which requires understanding the microstructure-topology-mechanical properties relationships in these scaffolds. IMDEA Materials is carrying out an exhaustive investigation of the material behaviour (see Figs. 2 and 3) of the porous scaffolds of the Mg WE43 to obtain values of maximum resistance to compression and cyclic stresses under similar conditions of an implanted specimen. This also includes the degradation in simulated body fluids (SBF), mechanical resistance in SBF, and in situ studies of material and deformation evolution during exposure to SBF using advanced X-ray tomography techniques.

This knowledge will provide information on the critical microstructural and geometric factors that control the resistance and degradation of the scaffolds and will allow proposing adequate post-processing treatments to improve these properties. In addition, the microstructural and geometric information will be used to develop numerical models of its mechanical response (Figure 2old), with a view to its future integration in models of mechanoregulation of growth and regeneration of bone tissue using porous alloy-based scaffolds.

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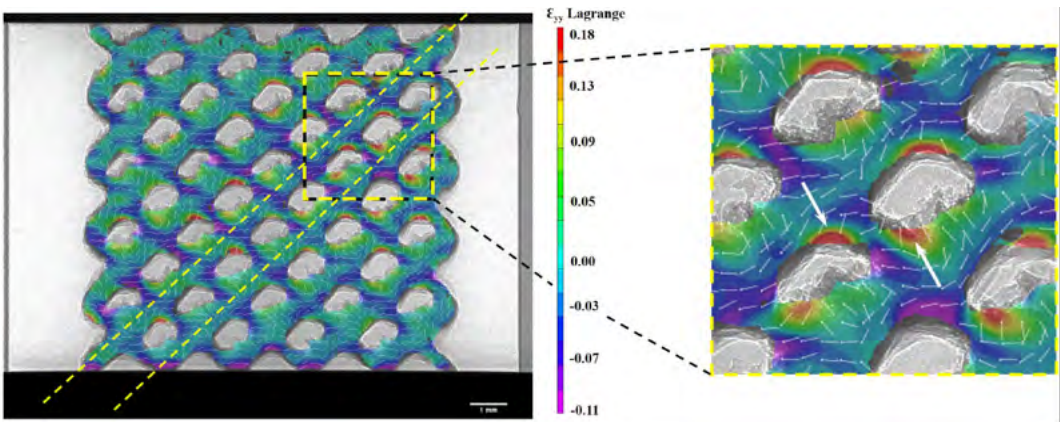


Fig. 3. Detail of DIC analysis during in-situ compression test of BCC scaffold (unpublished data)

Research highlights

In situ mechanical testing coupled with EBSD and high-resolution digital image correlation

Novel experimental tools are necessary to establish structure-property relationship of structural material for engineering applications. In particular, electron back-scattered diffraction (EBSD) and other techniques based on electron microscopy are extremely useful to reveal the microstructure features (grain boundaries, twin, precipitates) of polycrystalline solids.

However, the actual influence of these features on the deformation and fracture mechanisms can only be ascertained by means of in situ mechanical tests within the scanning electron microscope. To achieve these objectives, researchers at IMDEA Materials Institute have developed an experimental set-up that allows to superpose the microstructure evolution (by means of EBSD) with the strain distribution (by means of high-resolution digital image correlation, HR-DIC) during mechanical tests that are carried out within the chamber of the scanning electron microscope [1]. HR-DIC is a non-contact technique that is able to capture the strain distribution on the sample surface with a submicron resolution by tracking the movement of the features of a microscopic pattern deposited on the sample.

The experimental set-up is made up of a micromechanical testing machine that can be placed in a holder within the vacuum chamber of the scanning electron microscope (Fig. 1). If the holder is in the flat position, the sample is the machine is perfectly oriented for HR-DIC because the displacements of the pattern during deformation can be accurately captured by the secondary electrons (SE) detector in the microscope.

If a wedge is introduced between the mechanical testing machine and the holder, the sample is oriented at 50º that is the orientation to carry out EBSD (Fig. 1b). Moreover, a specific clamp was designed to hold the sample above the mechanical testing machine, so the electron beam scans the whole surface of the sample.

The displacement is applied to the same through motor and a double screw and a multi-gear system provides tension/compression along the central axis of the

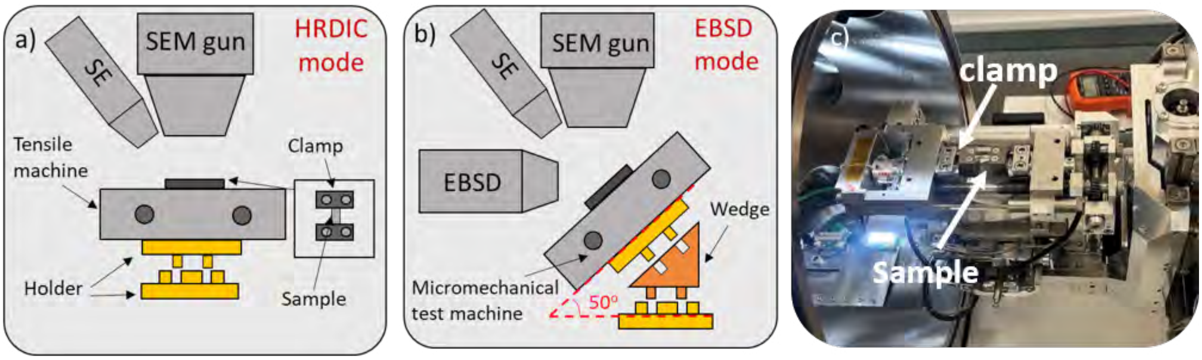


Fig. 1(a) schemic diagram of in-situ DIC imaging system. (b) Schematic diagram of in-situ EBSD system, (c) Photo of in-situ EBSD/HR-DIC mechanical test set-up.

specimens. The real time load-displacement curve can be recorded via the control system, and the mechanical test can be periodically stopped to acquire SE and EBSD images using an automated system to scan the whole surface of the sample.

This new in situ experimental set-up was used to study the interaction between twins and grain boundaries in Mg polycrystals. The orientation map of the polycrystalline Mg sample obtained by EBSD is plotted as a function of the applied tensile strain (1, 2 and 3%) in the top row of Fig. 2. The nucleation and growth of tensile deformation twins in different grains is clearly observed in these images.

In addition, the contour plots of the effective shear strain in the same region are plotted as a function of the tensile strain (1, 2 or 3%) in the same area in the bottom row of Fig. 2. The yellow slip lines indicate the activation of basal slip bands while the strain concentrations at the grain boundaries show the formation of dislocation pile-ups.

[1] M. Sarebanzadeh, B. Yang, E. Nieto-Valeiras, A. Orozco-Caballero, J. LLorca, *Symposium on Mechanical Response of Materials Investigated through Novel In-situ Experiments and Modeling*, TMS 2023 Annual Meeting & Exhibition, San Diego, California March 19th-23rd, 2023.

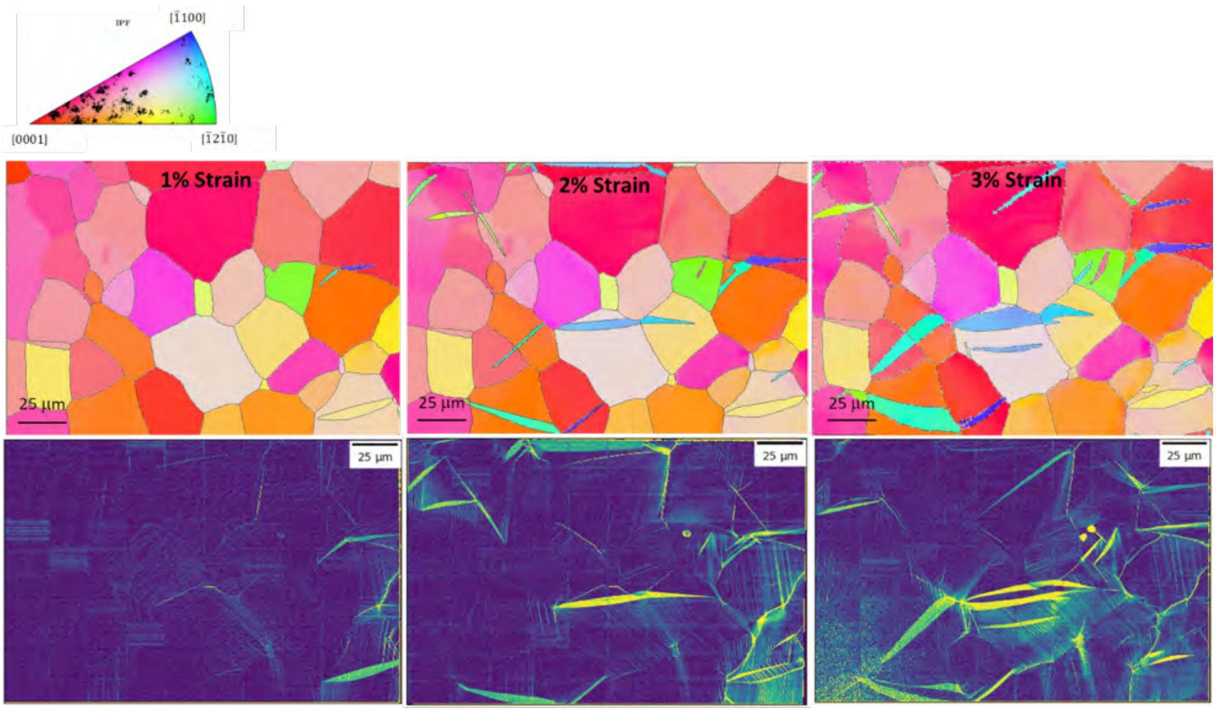


Fig. 2. EBSD maps (top row) and DIC maps (buttom row) for strain steps 1%, 2% and 3%.

Binder Jet green parts microstructure: advanced quantitative analysis

3D binder jet technology has drawn significant attention in recent years thanks to its ability to build complex shapes with a wide variety of commercial powders, together with the advantage of not using high energy sources during the printing process. Binder jet makes use of several printheads containing a formulated binder to build the layers of a part within a few seconds. This allows a significant improvement of the manufacturing productivity and quality with respect to laser powder bed fusion (LPBF) or conventional metal injection molding (MIM).

Current scientific and industrial investigations in binder jet are focused on the relationship between the printing parameters, the macroscopic properties, and the microstructures of sintered parts. However, there is a knowledge gap related to the relationship between the process parameters and the microstructure and properties of green parts.

In this work, a novel green microstructural analysis methodology, based on scanning electron microscopy (SEM) and X-ray computed tomography (XCT), is presented. SEM microstructural observations are supported by machine learning pixel-wise classification algorithms that enables image analysis. This new method facilitates the definition of green parts' key process metrics and the description of consolidation mechanisms (layer consolidation, powder bed interactions) under different printing conditions, before sintering. Thus, the binder and porosity distributions in green microstructures can be correlated to green and sintered macroscopic properties, such as sintered density,

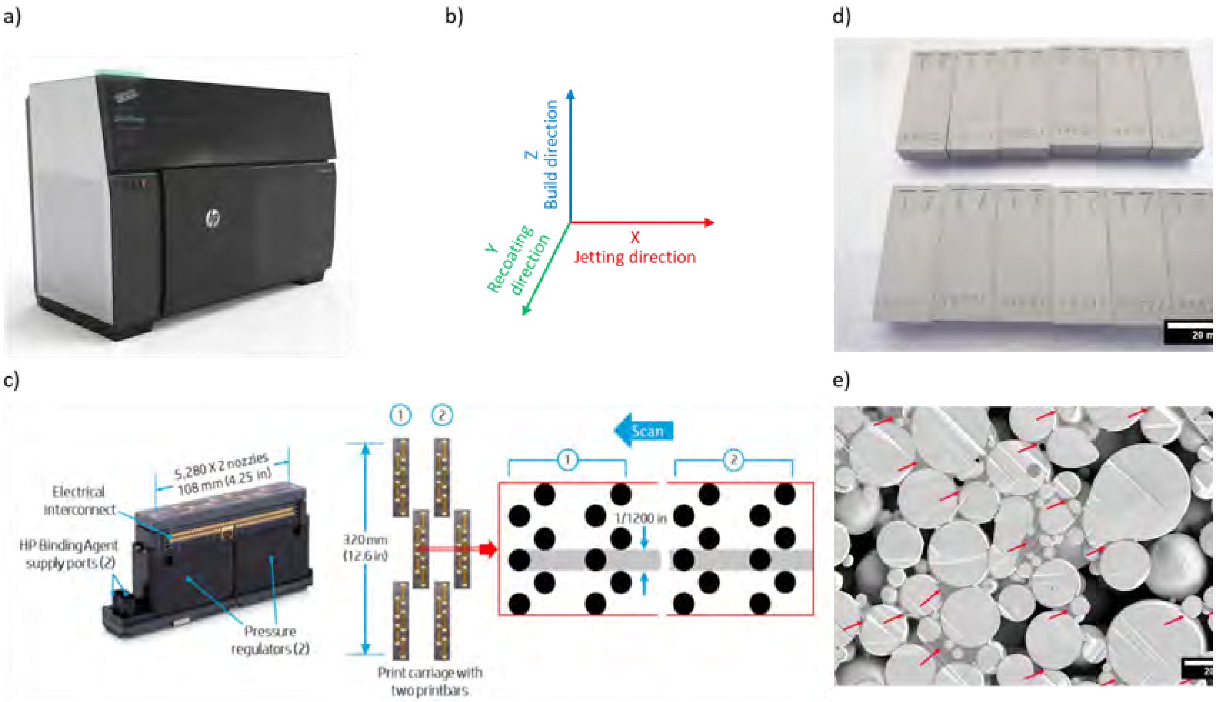


Fig. 1.3D Metal Jet a) Printer; b) Printer coordinate system; c) Thermal Inkjet Printhead and Printhead architecture; d) Green TRS bars; e) SEM micrograph from an Ion Beam Milling (IBM) green part cross section, red arrows indicate binder attaching metal particles.

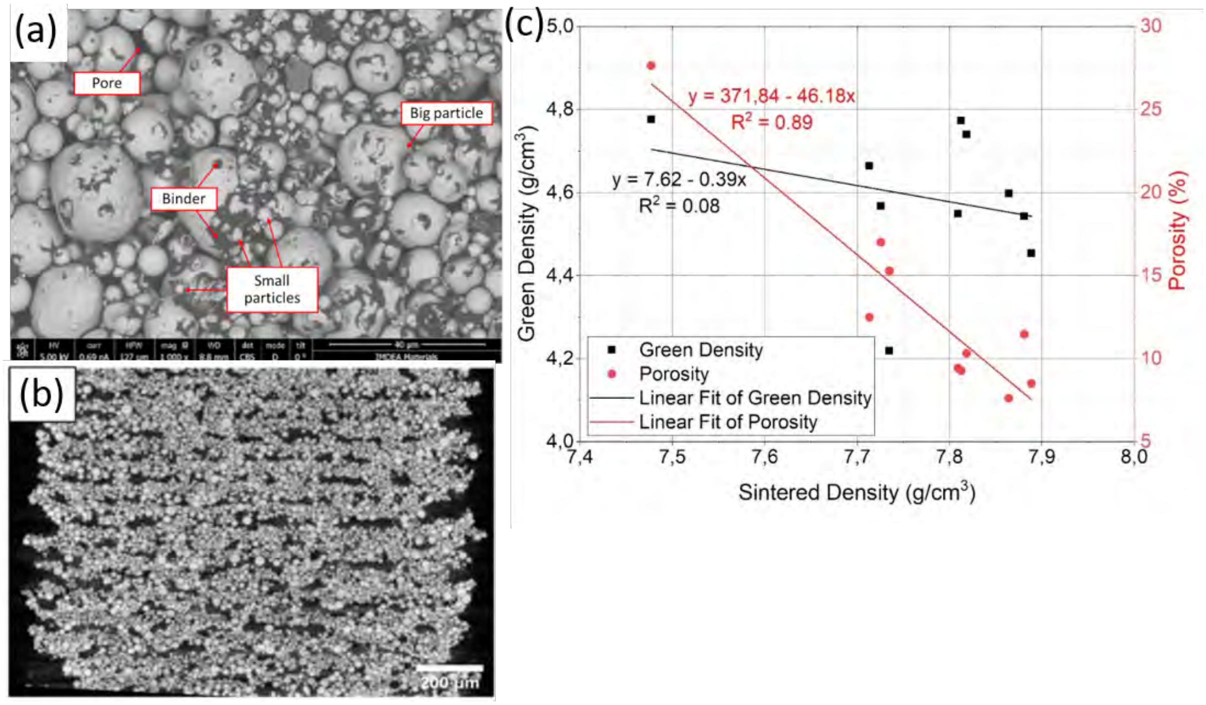


Fig. 2. (a) SEM micrographs showing binder distribution with darker contrast along the particles of a green part cross section. (b) XCT cross section in the printing direction showing the characteristic microstructure of the green part. (c) Relationship between green and sintered densities and porosity.

with a final modelling and prediction objective for process acceleration. The proposed novel and robust methodology is applied to particular empirical cases.

The selected material for the investigation was stainless steel (SS) 316L. SS-316L was gas-atomised to produce powder particles with a mean diameter of 13 µm. The manufactured parts were printed with an HP Metal Jet 3D printer, presented in Fig. 1a The employed coordinate system of the printer is shared in Fig. 1b HP Metal Jet system works with thermal inkjet printheads, formed by two carriages with 5280 nozzles each (Fig. 1c), working with a polymeric latex-based binder. Fig. 1d shows representative transverse rupture strength (TRS) bars and Fig. 1e a ion milling cross section of the green microstructure [1].

The SEM scanning parameters were optimised to perform automatic acquisition and analysis of the images and to obtain statistical relevant information as well as possible microstructural variations in the printing direction. Figure 3a illustrates an example of such an SEM micrograph. Binder is generally observed to be located between particles. Also, some particle surfaces show residual binder in the spots where they were joined before the cut preparation. Fig. 3b shows an XCT cross section showing the layering structures of the printing process. The image analysis with AI-based method was developed to extract the relevant parameters. The relationship between green and sintered densities and porosity was determined.

[1] S. Bafaluy Ojeda, J. Torrents-Barrena, M.T. Pérez-Prado, R. Muñoz Moreno, F. Sket. *Binder Jet green parts microstructure: advanced quantitative analysis*, J. Mater. Res. Technol., 23, 3974-3986, 2023.

principal investigators

Senior Researchers

Prof. José Manuel Torralba

Director. Sustainable Powder Metallurgy

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

Research Interests

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

Dr. Jon M. Molina-Aldareguia

Deputy Director. Micromechanics and Nanomechanics

Ph.D. in Materials Engineering from the University of Cambridge. UK.

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.

Prof. Javier LLorca

Scientific Director, Bio/Chemo/Mechanics of Materials

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

Professor of Materials Science, Technical University of Madrid

Research Interests

Development of new materials for engineering applications in transport, energy and health. The processing-structure-properties relationships of materials are established by means of different computational tools and multiscale modeling strategies as well as in situ and in operando characterisation techniques. Particular emphasis is given to the interaction among biological, chemical and mechanical processes. This information is used to design new materials that are manufactured by means of advanced processing techniques (including additive manufacturing of metallic alloys, polymers and composites, magnetron sputtering, etc.).

Dr. Johan Christensen

Senior Researcher, Acoustic and Mechanical Metamaterials.

Ph.D. in Condensed Matter Physics, Autonomous University of Madrid, Spain.

Research Interests

Theoretical description and numerical modelling of metamaterials and topological insulators.The investigation comprises the exploration of novel material properties and physical effects, both in the context of wave propagation, as well as topology induced deformations and wave guiding. The driving force is predominantly to nurture fundamental science but technological implications are also targeted.

Prof. Carlos González

Senior Researcher, Structural Composites

Ph.D. in Materials Science from the 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 optimisation.

Dr. Maciej Haranczyk

Senior Researcher,
Computational and Data-Driven Materials Discovery

Ph.D. in Chemistry from the 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. Srdjan Milenkovic

Senior Researcher,
Solidification Processing & Engineering

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

Research Interests

Advanced solidification processing techniques (centrifugal and suction casting, reactive infiltration) with special emphasis on small scale gas atomisation 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. María Teresa Pérez-Prado

Senior Researcher,
Sustainable Metallurgy

Ph.D. in Materials Science from the 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 recrystallisation mechanisms of light and high temperature metals; fabrication of novel metallic phases with improved mechanical and functional properties by non-equilibrium processing.

Prof. Ignacio Romero

Senior Researcher,
Computational Solid Mechanics

Ph.D. in Civil Engineering, from the 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. Ilchat Sabirov

Senior Researcher,
Physical Simulation

Ph.D. in Metallurgy from Montanuniversitaet Leoben. Austria

Research Interests

Physical simulation of metallurgical processes, their optimisation 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. Javier Segurado

Senior Researcher,
Multiscale Materials Modelling

Ph.D. in Materials Engineering from the 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 homogenisation 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. Federico Sket

Senior Researcher, In-situ processing and mechanical 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

Senior 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.

Researchers

Dr. Juan José Vilatela

Senior Researcher, Multifunctional Nanocomposites

Ph.D. in Materials Science from the University of Cambridge. UK.

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. 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 environmentally 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. Jennifer Patterson

Researcher, Biomaterials and Regenerative Medicine

Ph.D. in Bioengineering from the University of Washington, USA

Research Interests

Synthesis of novel biomaterials, with a particular focus on hydrogels; processing of biomaterials into complex 3D structures; characterisation of the physical and chemical properties of biomaterials; evaluation of cytocompatibility and biological functionality in vitro; preclinical evaluation in small animal models in vivo; tissue engineering applications; development of 3D in vitro tissue models and organ-on-chip devices.

Visiting Scientists

Prof. Thomas Bieler
Visiting Researcher

Ph.D. in Materials Science from the University of California, Davis, USA.

Professor, Chemical Engineering and Materials Science, Michigan State University, USA.

Prof. Douglas Spearot
Visiting Researcher

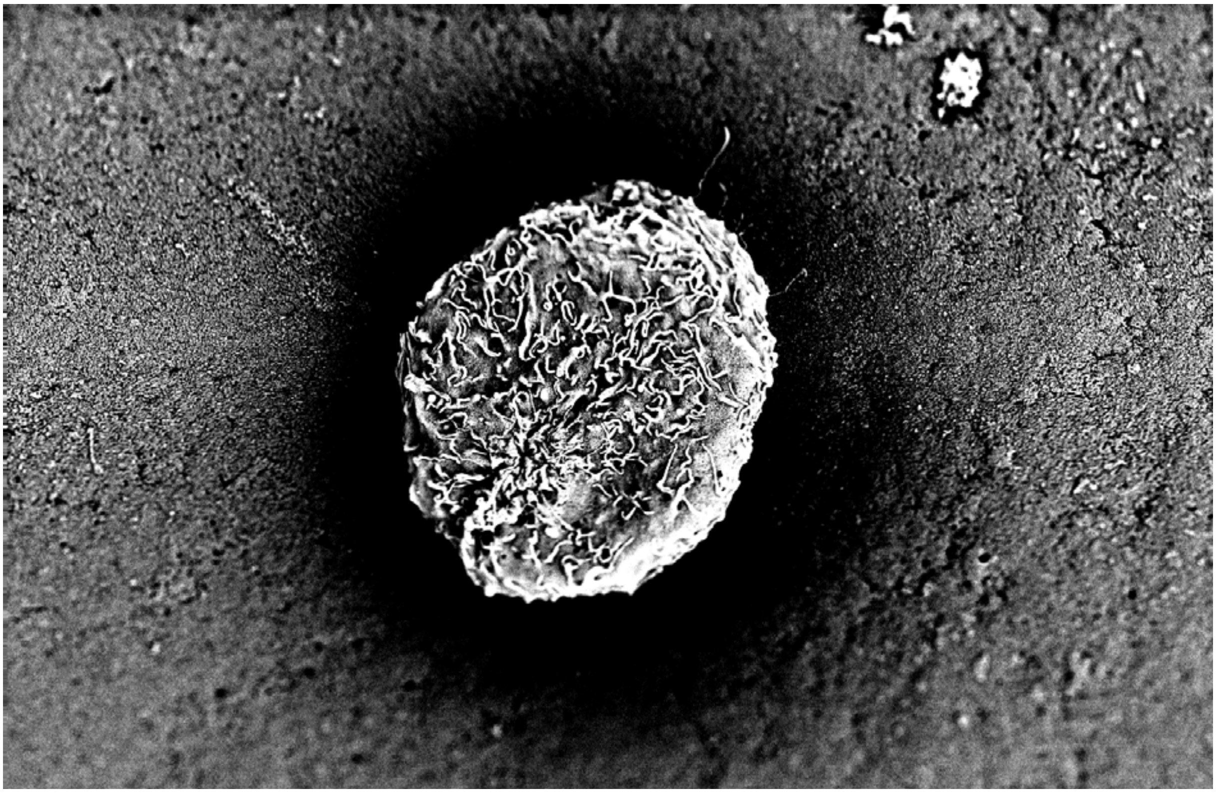
Ph.D. in Mechanical Engineering from the Georgia Institute of Technology, USA.

Professor, Department of Mechanical & Aerospace Engineering, Herbert Wertheim College of Engineering at the University of Florida, USA.

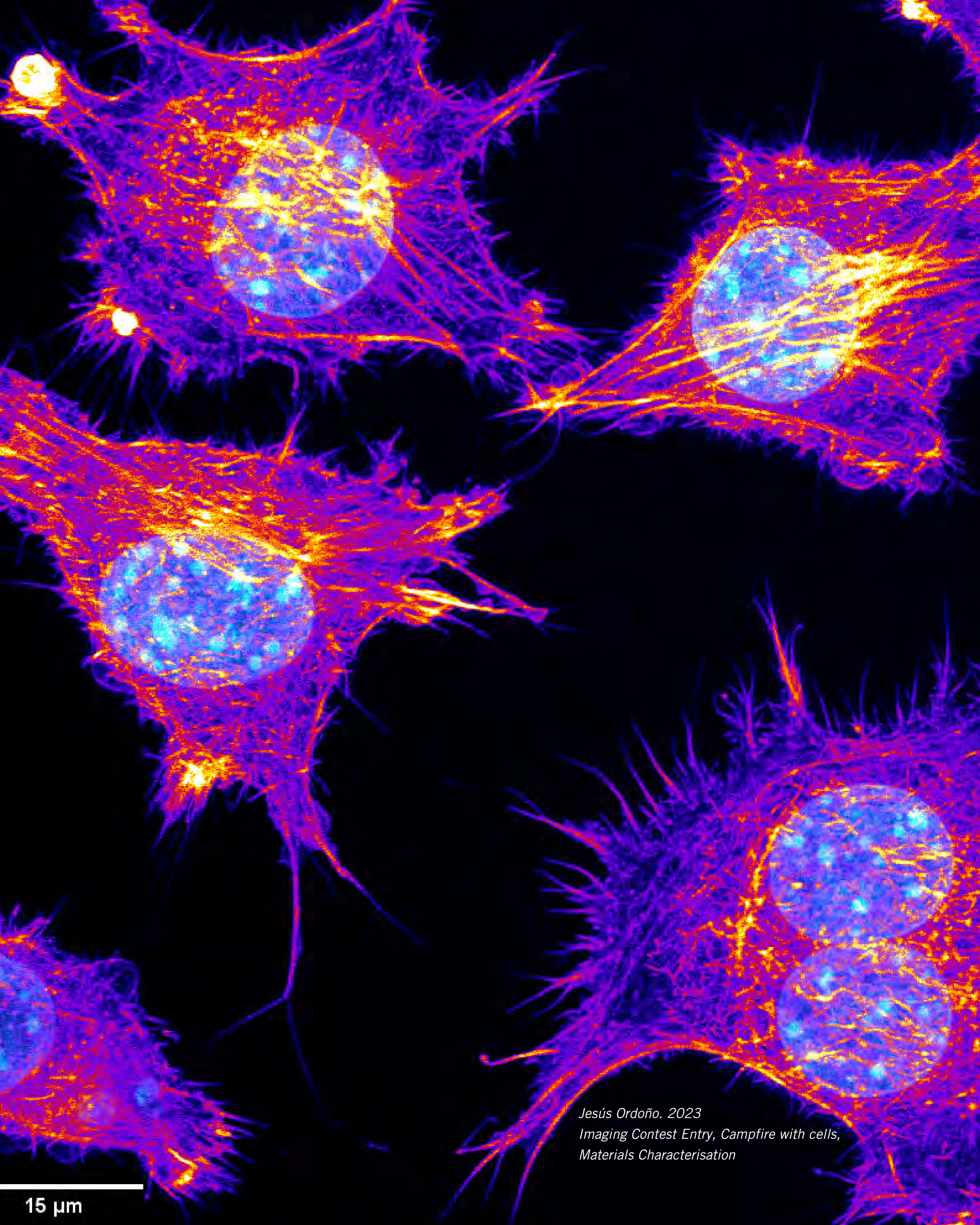
Prof. Jaime Marian
Visiting Researcher

Ph.D. in Mechanical Engineering from the Technical University of Madrid, Spain.

Professor of Mechanical and Aerospace Engineering at the University of California, USA.



Shuanglan Du. 2023 Imaging Contest Entry,
Beginning of Life, Materials Characterisation.



Jesús Ordoño. 2023
Imaging Contest Entry, Campfire with cells,
Materials Characterisation

annex

R&D projects and contracts 67

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1. R&D projects and contracts

1.1. European R&D Projects (European Commission)

Title/Acronym: Universal processing route for high-performance nanostructured yarns/ UNIYARNS
Partners: IMDEA Materials Institute
Period: 2022 - 2027
Funding Institution/Programme: European Commission/Horizon Europe Programme – ERC Consolidator Grant
Principal Investigator: Dr. J.J. Vilatela

Title/Acronym: Mechanics of Nanoporous W under irradiation/MENAWIR
Partners: IMDEA Materials Institute
Period: 2022 - 2024
Funding Institution/Programme: European Commission/Horizon Europe Programme – Marie Skłodowska-Curie Actions – PF
Principal Investigator: Dr. C. Ruestes; Supervisor: Prof. J. Segurado

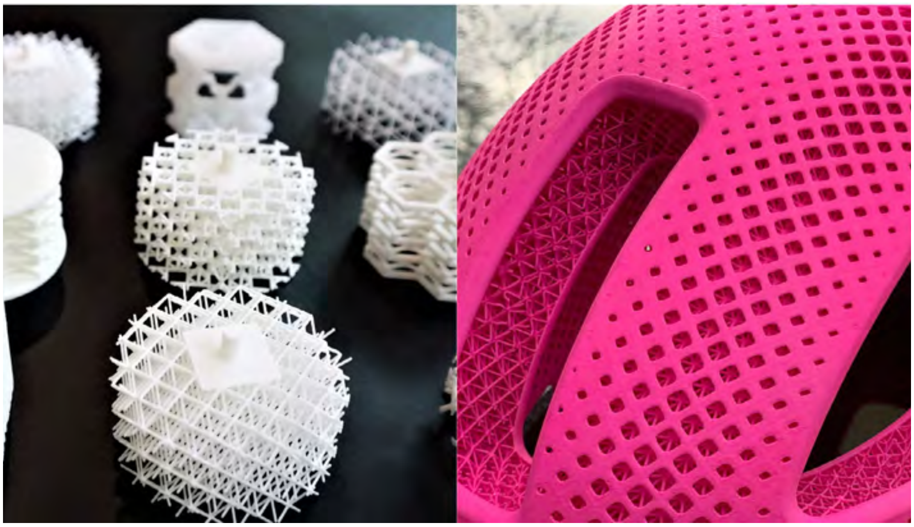
Title/Acronym: Resource-efficient steel construction using additive manufacturing/ CONSTRUCTADD
Partners: The Politecnico di Milano (Coordinator), IMDEA Materials Institute, RWTH Aachen University, the University of Pisa, Prima Industrie, Vallourec, Mimete, Cimolai, ArcelorMittal, BLM and DNV Netherlands
Period: 2022 - 2026
Funding Institution/Programme: European Commission/Research Fund for Coal and Steel (RFCS)
Principal Investigator: Dr. I. Sabirov

A 3D-printed steel plate. CONSTRUCTADDseeks to improve resource efficiency in the steel construction sector through the use of additive manufacturing.

Title/Acronym: Smart 4D biodegradable metallic shape-shifting implants for dynamic tissue restoration/BIOMET4D
Partners: IMDEA Materials Institute (Coordinator), the Technical University of Madrid, Aerosint, Meotec, the University Hospital Cologne, the National University of Ireland Galway and the Gregorio Marañón Hospital Biomedical Research Foundation
Period: 2022 - 2026
Funding Institution/Programme: European Commission/Horizon Europe Programme – EIC Pathfinder Open
Principal Investigator: Dr. J. Patterson

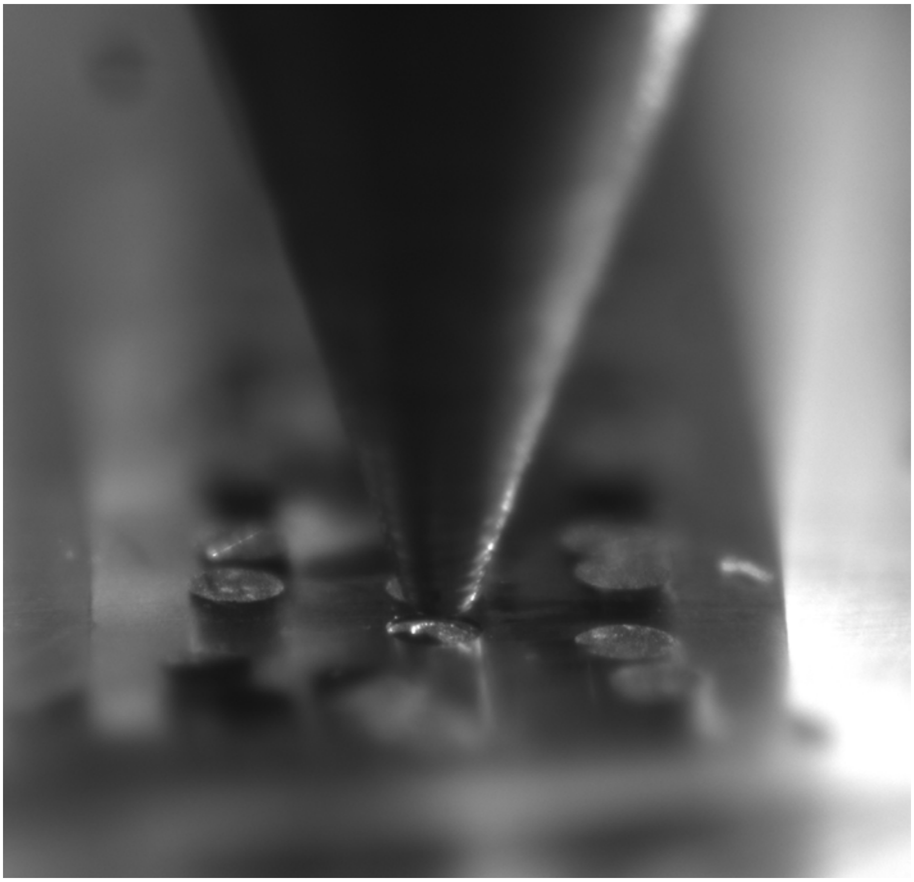
Title/Acronym: Additive manufacturing of amorphous metals for soft magnetics/AM2SOFTMAG
Partners: Saarland University, IMDEA Materials Institute, the Italian National Institute of Metrology Research and Heraeus
Period: 2022 - 2026
Funding Institution/Programme: European Commission/Horizon Europe Programme – EIC Pathfinder Open
Principal Investigator: Dr. M. T. Pérez-Prado

Title/Acronym: Study and understanding of gas phase entangled reactions for yarn assembly via robust nanomaterial aerogelation/SUPERYARN
Partners: IMDEA Materials Institute
Period: 2022 - 2023
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie Actions – IF
Principal Investigator: Dr. M. Vázquez; Supervisor: Dr. J.J. Vilatela



The MOAMMM Project aims to develop a data-driven design methodology for additively manufactured mechanical components made of metamaterials and to design and optimise shock-absorption devices, such as the helmet pictured here.

This image, taken by José Luís Jímenez, shows a push out test carried out on in an Instron universal mechanical testing machine on magnesium fibres of 300 microns in diameter as part of the BIOIMPLANT project.



Title/Acronym: Development of gamma prime strengthened CoNi superalloy for advanced sustainable manufacturing technologies/CNSTECH
Partners: IMDEA Materials Institute
Period: 2021 – 2023
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie Actions – IF
Principal Investigator: Dr. A. Mohammadzadeh; Supervisor: Prof. J. M. Torralba

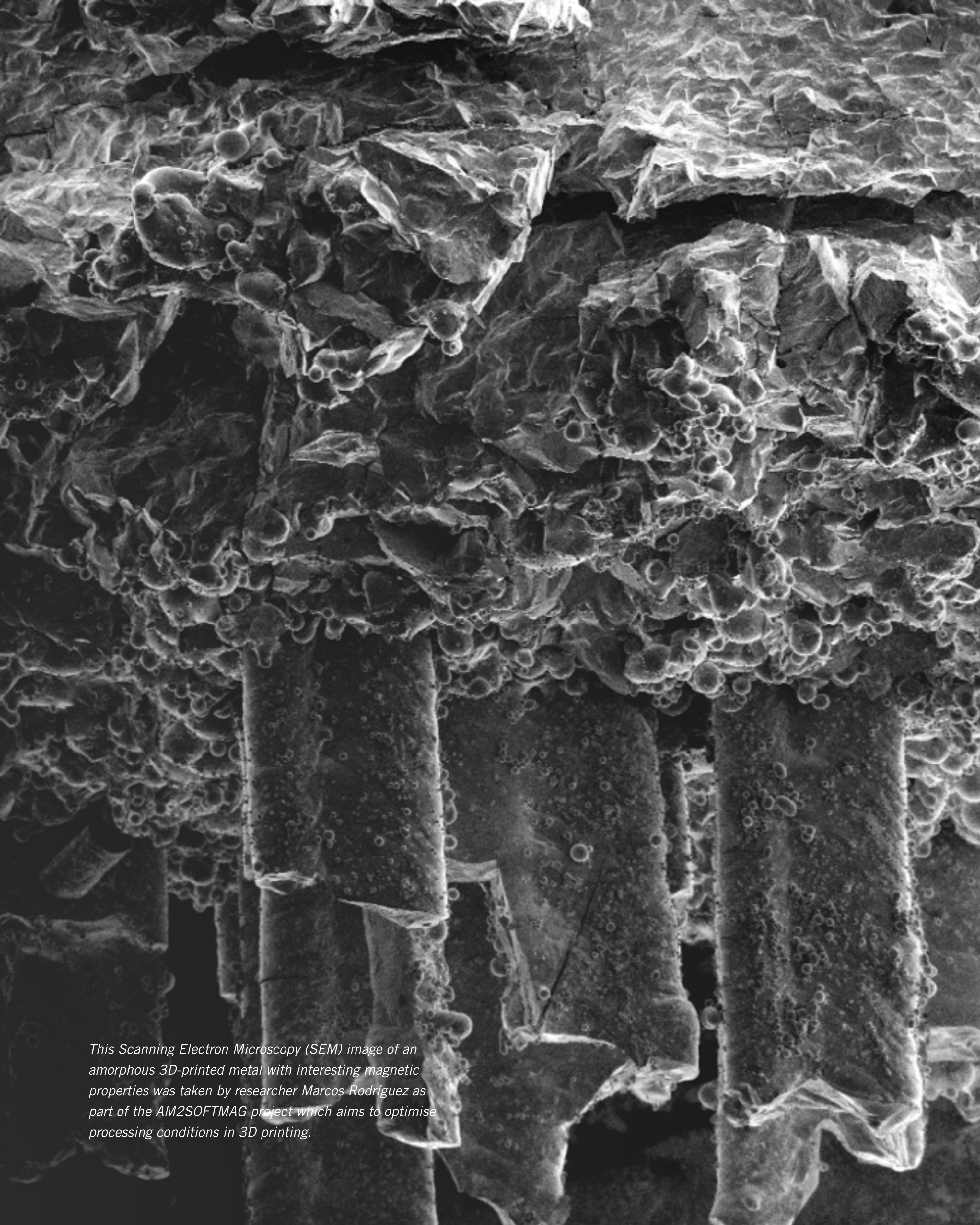
Title/Acronym: Digital method for improved manufacturing of next-generation multIfunctIonal airframe parts/DOMMINIO
Partners: AIMEN (Coordinator), IMDEA Materials Institute, Tortech Nano Fibers, IRES, the National Technical University of Athens, Aciturri Engineering, IPC, BAE Systems, EASN, ESI Group, Arts et Métiers, INCAS and Dasel
Period: 2021 - 2024
Funding Institution/Programme: European Commission/Horizon 2020 Programme - Societal Challenges - Smart, Green And Integrated Transport
Principal Investigators: Prof. C. González and Dr. J.J. Vilatela

Title/Acronym: European database for multiscale modelling of radiation damage/ ENTENTE
Partners: CIEMAT (Coordinator), IMDEA Materials Institute, Bay Zoltan Nonprofit Ltd. for Applied Research (BZN), the French Alternative Energies and Atomic Energy Commission (CEA), CNRS, Electricité de France (EDF), Framatome, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), the Institute for Radiological Protection and Nuclear Safety (IRSN), the KTH Royal Institute of Technology in Stockholm, the University of Cantabria, National Nuclear Laboratory Limited (NNL), Phimeca, SCK CEN, the University of Warwick, the University of Bristol, the Materials Performance Centre of the University of Manchester, the University of Alicante, the Technical University of Catalunya - BarcelonaTech, the Technical University of Madrid, the Culham Centre for Fusion Energy, UJV Rez, the VTT Technical Research Centre of Finland, State Enterprise State Scientific and Technical Center for nuclear and radiation safety (SSTC), Chalmers University of Technology and the Central Research Institute of Electric Power Industry (CRIEPI)
Period: 2020 - 2024
Funding Institution/Programme: European Commission/EURATOM
Principal Investigators: Drs. J.M. Molina-Aldareguia and M. Monclús

Title/Acronym: Tailored lightweight sandwich composites with multifunctional properties and good designability/TESCOM
Partners: IMDEA Materials Institute
Period: 2020 – 2022
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie Actions – IF
Principal Investigator: Dr. X. Lin; Supervisor: Dr. D-Y Wang

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

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

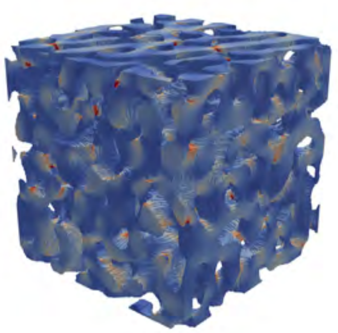


This Scanning Electron Microscopy (SEM) image of an amorphous 3D-printed metal with interesting magnetic properties was taken by researcher Marcos Rodríguez as part of the AM2SOFTMAG project which aims to optimise processing conditions in 3D printing.

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

Title/Acronym: Multi-scale optimisation for additive manufacturing of fatigue resistant shock-absorbing metamaterials/MOAMMM
Partners: The University of Liège (Coordinator), IMDEA Materials Institute, KU Leuven, Johannes Kepler University Linz and CIRP
Period: 2020 - 2024
Funding Institution/Programme: European Commission/Horizon 2020 Programme – FET Open
Principal Investigators: Prof. J. Segurado and Dr. M. Monclús

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



This image, generated by Carlos Ruestes, shows stress distribution on nanoporous tungsten under tension. Simulation performed with FFTMAD as part of the MeNaWir project.

Title/Acronym: European Training Network to develop improved bioresorbable materials for orthopaedic and vascular implant applications/ BIOIMPLANT ITN
Partners: The National University of Ireland Galway (Coordinator), IMDEA Materials Institute, the Queens University of Belfast, RWTH Aachen, Boston Scientific, 3D Technology, Vascular Flow Technologies, Meotec and ITA Textile Technology Transfer
Period: 2018 - 2022
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie Actions - ITN
Principal Investigator: Prof. J. LLorca

1.2. Other International R&D Projects

Title/Acronym: Exploiting low-dimensional properties of carbon nanotubes in macroscopic yarns for charge transfer and storage/NANOYARN
Partners: IMDEA Materials Institute
Period: 2018 – 2022
Funding Institution/Programme: The Air Force Office of Scientific Research (AFOSR)
Principal Investigator: Dr. J.J. Vilatela

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

1.3. National R&D Projects

Title/Acronym: Implantable device for brain tumor treatment using electrical fields/ DITTCE
Partners: The Technical University of Madrid (Coordinator), IMDEA Materials Institute, the Institute of Health Carlos III, Niño Jesús Hospital Biomedical Research Foundation, La Princesa University Hospital Biomedical Research Foundation and Insyte
Period: 2022 - 2025
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Strategic Lines
Principal Investigator: Dr. M. Echeverry

Title/Acronym: Nanostructure network electrodes to realise the high energy density 3b/4a battery/MAT4BAT
Partners: IMDEA Materials Institute
Period: 2022 - 2024
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Green and Digital Transition
Principal Investigator: Dr. J.J. Vilatela

Title/Acronym: Biobased flame retardant system for sustainable polymers: molecule design, digital synthesis, digital analysis, data-driven approach/DIGIBIOFOAM
Partners: IMDEA Materials Institute
Period: 2022 - 2024
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Green and Digital Transition
Principal Investigator: Drs. D-Y Wang and M. Haranczyk

Title/Acronym: Consolidation and study of behavior under hydrogen/NATURE
Partners: Carlos III University of Madrid (Coordinator), IMDEA Materials Institute and the Technical University of Madrid
Period: 2022 - 2024
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Green and Digital Transition
Principal Investigator: Dr. S. Milenkovic

Title/Acronym: High-throughput strategies for the discovery of new catalysts for the hydrogen economy through elastic strain engineering/CATBYESE
Partners: IMDEA Materials Institute
Period: 2022 - 2024
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Green and Digital Transition
Principal Investigator: Prof. J. LLorca

Title/Acronym: Porous metal genomics for tailoring mechanical properties of light-weight 3D-printed architectures/PORMETALOMIOCS
Partners: IMDEA Materials Institute (Coordinator), Institute of Mathematics of the Polish Academy of Sciences and Technion
Period: 2022 - 2025
Funding Institution/Programme: Spanish Ministry of Science and Innovation - European Commission/M-ERA.Net
Principal Investigator: Dr. M. Haranczyk

Title/Acronym: Synthesis and assembly of long metal oxide nanowires for energy/SALMONE
Partners: IMDEA Materials Institute
Period: 2022 - 2026
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Knowledge Generation
Principal Investigator: Drs. J.J. Vilatela, D. Tourret and A. Pendashteh

Title/Acronym: Design of master alloys for sintered steels/DAMAS
Partners: AMES (Coordinator), IMDEA Materials Institute and the Carlos III University of Madrid
Period: 2022 - 2025
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Public-Private Collaboration
Principal Investigator: Dr. D. Tourret

Title/Acronym: Micro/macro-modeling of solidification in additive manufacturing/ MIMMOSA
Partners: IMDEA Materials Institute
Period: 2022 - 2024
Funding Institution/Programme: Spanish Ministry of Science and Innovation/ International joint programming actions (seal of excellence European Commission/ Horizon 2020 Programme – Marie Skłodowska-Curie Actions – IF)
Principal Investigator: Dr. R. Tavakoli; Supervisor: Dr. D. Tourret

Title/Acronym: Two-dimensional disruptive materials for the new technological transformation\MAD2D
Partners: Complutense University of Madrid (Coordinator), IMDEA Materials Institute, IMDEA Energy Institute, the autonomous University of Madrid and the Techncial University of Madrid
Period: 2022 - 2025
Funding Institution/Programme: Spanish Ministry of Science and Innovation - Regional Government of Madrid/Complementary R&D&I plans-REACT EU resources
Principal Investigators: Prof. J. LLorca and Drs. J.J. Vilatela and M. Haranczyk

Title/Acronym: Biobased, self-reinforced and flame-resistant all-solid-state polymer electrolytes for new generation fire-safe battery/BIOFIRESAFE
Partners: IMDEA Materials Institute
Period: 2021 - 2024
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Research Challenges
Principal Investigator: Dr. D-Y Wang

Title/Acronym: X-ray microtomograph with capacity for in situ testing and laboratory-based diffraction contrast tomography/LAB-BASED DCT
Partners: IMDEA Materials Institute
Period: 2021 - 2023
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Scientific and Technical Infrastructures and Equipment
Principal Investigator: Dr. F. Sket

Title/Acronym: European Project Office (OPE) IMDEA Materials Institute 2021-2022
Partners: IMDEA Materials Institute
Period: 2021 - 2022
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Europe Networks and Managers - Europa Technology Centres
Coordinator: Miguel Ángel Rodiel

Title/Acronym: Advanced materials and nanomaterials Spanish technological platform 2021-2022 /MATERPLAT 2021-2022
Partners: IMDEA Materials Institute (Technical Secretariat)
Period: 2021 – 2022
Funding Institution/Programme: Spanish Ministry of Science and Innovation/ Technological Platforms
Coordinator: Miguel Ángel Rodiel

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

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

Title/Acronym: Development of multi-material and multifunctional 3D parts through additive manufacturing assisted by intelligent material and process design/MULTI-FAM
Partners: Arcelor Mittal (Coordinator), IMDEA Materials Institute and AIMEN
Period: 2020 - 2022
Funding Institution/Programme: Spanish Ministry of Science and Innovation/ Collaboration Challenges
Principal Investigators: Dr. I. Sabirov and Dr. D. Tourret

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

Title/Acronym: Scanning electron microscope with field emission source for characterisation of materials with EDX and EBSD/FEGSEM
Partners: IMDEA Materials Institute
Period: 2019 - 2022
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Scientific and Technical Infrastructures and Equipment
Principal Investigator: Dr. J.M. Molina-Aldareguia

Title/Acronym: Design of electron transfer in semiconductor-dye hybrid nanoparticles for low-temperature solar cells/HYNANOSC
Partners: The Universiity of Alicante (Coordinator) and IMDEA Materials Institute
Period: 2019 - 2021
Funding Institution/Programme: Spanish Ministry of Economy and Competitiveness/ Research Challenges
Principal Investigator: Dr. J.J. Vilatela

Title/Acronym: Grain Boundaries in Hexagonal microstructures: Linking processing and properties in lightweight structural alloys - HexaGB
Partners: IMDEA Materials Institute (Coordinator) and the Technical University of Madrid
Period: 2019 – 2022
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Research Challenges
Principal Investigator: Dr. D. Tourret

1.4. Regional R&D Projects

Title/Acronym: Design and scaling of new hard coatings deposited by HiPIMS for high-speed milling/ HIPDUR
Partners: NANO4ENERGY and IMDEA Materials Institute
Period: 2022 - 2025
Funding Institution/Programme: Regional Government of Madrid/Industrial Doctorate
Principal Investigator and Supervisor: Dr. M. Monclús; Doctoral Researcher: A. García

Title/Acronym: Metamaterial printing using shape memory alloys and functional gradients for a new generation of smart implants/i-MPLANTS-CM
Partners: The Technical University of Madrid and IMDEA Materials Institute
Period: 2021 - 2024
Funding Institution/Programme: Regional Government of Madrid/Synergy projects
Principal Investigator: Dr. J.M. Molina-Aldareguia

Title/Acronym: Materials and models against pandemics/MAMAP-CM
Partners: IMDEA Materials Institute
Period: 2021 - 2022
Funding Institution/Programme: Regional Government of Madrid/REACT EU
Principal Investigator: Prof. J. LLorca

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

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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
Principal Investigator and Supervisor: Dr. M. Haranczyk; Doctoral Researcher: G. Lo Dico

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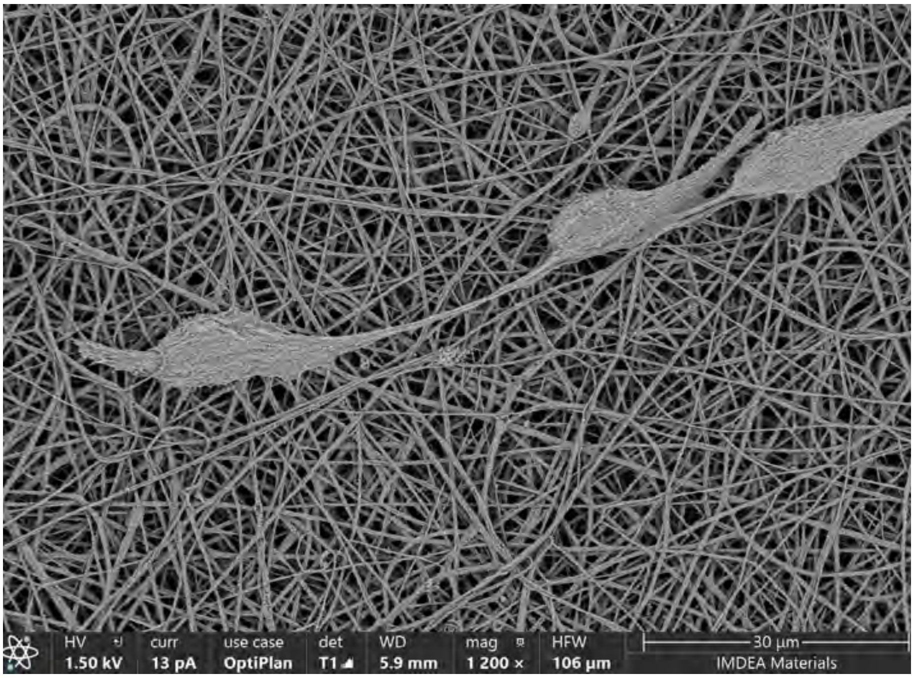

"This image, taken by Patricia Paramio as part of the MAMAP-CM project, shows BEAS-2B bronchial epithelium cells seeded on Nylon membranas."

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
Principal Investigators and Supervisors: Drs. J.M. Molina-Aldareguia and M. Monclús; Doctoral Researcher: A. Méndez

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

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

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

1.5. Privately-funded R&D Projects

Title/Acronym: Design and scaling of new hard coatings deposited by HiPIMS for high-speed milling/ HIPDUR
Company: NANO4ENERGY
Period: 2022 - 2025
Principal Investigator: Dr. M. Monclús

Title/Acronym: Smart, adaptive and sustainable technologies for agile, zero-defect manufacturing of composite materials by resin transfer process\SM@RTM
Company: IDAERO Solutions
Period: 2022 - 2024
Principal Investigator: Prof. C. González

Title/Acronym: Carbon nanotube fabrics for displacement of metallic current conductors in the next generation Li-ion batteries/NANOCARBAT2
Company: RICE University
Period: 2022 - 2023
Principal Investigator: Dr. J.J. Vilatela

Title/Acronym: Computed tomography inspection/XCTVSUS
Company: Airbus Operations
Period: 2022-2023
Principal Investigator: Dr. F. Sket

Title/Acronym: Evaluating the potential of high-entropy alloys elaborated by powder metallurgy for horology applications/HEAH
Company: Rolex
Period: 2022-2023
Principal Investigator: Prof. J. M. Torralba

Title/Acronym: Microstructural and mechanical characterisation of hard coatings/ MICROATING
Company: NANO4ENERGY
Period: 2022-2023
Principal Investigator: Dr. J.M. Molina-Aldareguia

Title/Acronym: Investigation of the properties of lightweight materials for high-altitude pseudo-satellite/HIPSET
Company: SMARTHAPS
Period: 2022
Principal Investigator: Dr. D-Y Wang

Title/Acronym: Advice for The Shanghai Research Institute of Chemical Technology/ CONSULT
Company: Shanghai Research Institute of Chemical Technology
Period: 2022-2023
Principal Investigator: Dr. D-Y Wang

Title/Acronym: High-performance CNT fibre development through mechanical study of CNT bundles/NANOBUNDLE II
Company: TOYOTA Motor Europe
Period: 2021-2022
Principal Investigator: Dr. J.J. Vilatela

Title/Acronym: Evaluation of the potential application of earth oxide in flame retardant/ REOCABLE
Company: The Baotou Research Institute of Rare Earths
Period: 2021 - 2022
Principal Investigator: Dr. D-Y Wang

Title/Acronym: Carbon nanotube fabrics for displacement of metallic current conductors in the next-generation Li-ion batteries/NANOCARBAT
Company: RICE University
Period: 2021 - 2022
Principal Investigator: Dr. J.J. Vilatela

"This image, taken by José Luis Jiménez as part of the BINOMIAL project, shows three composite sandwich panels impacted samples at different energies."

Title/Acronym: Optimisation of the processing route of polyurethane-coated composite material/NEOTAIL
Company: 3M España
Period: 2021 - 2024
Principal Investigator: Prof. C. González

Title/Acronym: Nanoporous Material Genome Center/MNGC
Company: University of Minnesota
Period: 2020-2022
Principal Investigator: Dr. M. Haranczyk

Title/Acronym: Improvement of the 3D Metal Jet Part Quality through print mode development supported by HR-XCT characterisation of the printed parts/METAL JET XCT
Company: HP Printing and Computing Solutions
Period: 2020 - 2022
Principal Investigators: Drs. M.T. Pérez-Prado and F. Sket

Title/Acronym: Evaluation of damage made by ballast impact in composite materials/ BINOMIAL
Company: Patentes TALGO
Period: 2019-2023
Principal Investigator: Prof. C. González

2. Fellowships

2.1. International

Programme: China Scholarship Council fellowships
Project: Intrinsic white emitting materials for lighting
Period: 2018-2022
Funding Institution: China Scholarship Council
Y. Duan

Programme: China Scholarship Council fellowships
Project: Functional properties of polymeric fabrics
Period: 2019-2023
Funding Institution: China Scholarship Council
X. Li

Programme: China Scholarship Council fellowships
Project: Fire behaviours of composite materials
Period: 2020-2024
Funding Institution: China Scholarship Council
X. Ao

Programme: China Scholarship Council fellowships
Project: Construction and mechanism of flame retardant with dynamic reversible covalent bond based on wood-plastic interface
Period: 2021-2022
Funding Institution: China Scholarship Council
C. H. Ding

Programme: China Scholarship Council fellowships
Project: New generation biodegradable polymers in tissue engineering
Period: 2021-2025
Funding Institution: China Scholarship Council
Y. Liu

Programme: China Scholarship Council fellowships
Project: New generation fire-retardant materials for Lithium-ion battery
Period: 2021-2025
Funding Institution: China Scholarship Council
M. Zhang

Programme: China Scholarship Council fellowships
Project: Marine-derived chitosan-based thermosensitive hydrogels and their applications in anti-ageing
Period: 2021-2025
Funding Institution: China Scholarship Council
S. Du

Programme: China Scholarship Council fellowships
Project: New generation environmentally friendly halogen-free flame retardant with combination of N-substituted alkoxy hindered amines
Period: 2021-2025
Funding Institution: China Scholarship Council
W. Ye

2.2. National

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

Programme: Ramón y Cajal
Period: 2021-2026
Funding Institution: Spanish Ministry of Science and Innovation
Dr. D. Tourret

Programme: Juan de la Cierva
Period: 2021-2022
Funding Institution: Spanish Ministry of Science and Innovation
Dr. M. Echeverry

Programme: Juan de la Cierva
Period: 2022-2024
Funding Institution: Spanish Ministry of Science and Innovation
Dr. JM. Guevara

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

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

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

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

Programme: Predoctoral Fellowships
Period: 2021-2025
Funding Institution: Spanish Ministry of Science and Innovation
D. Martín

Programme: Predoctoral Fellowships
Period: 2021-2025
Funding Institution: Spanish Ministry of Science and Innovation
I. Rodríguez

Programme: Predoctoral Fellowships
Period: 2021-2025
Funding Institution: Spanish Ministry of Science and Innovation
J. García

Programme: Predoctoral Fellowships
Period: 2021-2025
Funding Institution: Spanish Ministry of Science and Innovation
M. Castillón

Programme: Predoctoral Fellowships
Period: 2021-2025
Funding Institution: Spanish Ministry of Science and Innovation
I. Olaya

Programme: Sabbatical stays of foreign lecturers and researchers
Period: 2022
Funding Institute: Ministerio de Ciencia, Innovación y Universidades
D. Wang

Programme: Grants for pre-doctoral contracts for the training of Ph.Ds.
Period: 2022 - 2026
Funding Institute: Ministerio de Ciencia e Innovación
J. Redondo

Programme: Grants for pre-doctoral contracts for the training of Ph.Ds.
Period: 2022 - 2026
Funding Institute: Ministerio de Ciencia, Innovación y Universidades
B. Ozdemir

2.3. Regional

Programme: Talent Attraction Programme – Modality 1
Period: 2018-2023
Funding Institution: Madrid Regional Government
Dr. A. Ma

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

Programme: Youth Employment Programme/Research assistants and laboratory technicians
Period: 2021-2023
Funding Institution: Madrid Regional Government
G. Domínguez

Programme: Youth Employment Programme/Research assistants and laboratory technicians
Period: 2021-2023
Funding Institution: Madrid Regional Government
J. Espinoza

Programme: Youth Employment Programme
Period: 2022 - 2024
Funding Institute: Comunidad de Madrid
A. Vicente

Programme: Talent attraction programme
Period: 2022 - 2023
Funding Institute: Comunidad de Madrid
Anxin Ma

Programme: Programme I Investigate
Period: 2022-2023
Funding Institute: Comunidad de Madrid
J. León

Programme: Programme I Investigate
Period: 2022 - 2023
Funding Institute: Comunidad de Madrid
A. Pascual

Programme: Programme I Investigate
Period: 2022 - 2023
Funding Institute: Comunidad de Madrid
Name: P. Williams

Programme: Programme I Investigate
Period: 2022 – 2023
Funding Institute: Comunidad de Madrid
V. López

Programme: Programme I Investigate
Period: 2022-2023
Funding Institute: Comunidad de Madrid
A. Montero

Programme: Programme I Investigate
Period: 2022-2023
Funding Institute: Comunidad de Madrid
C. Corchado

Programme: Programme I Investigate
Period: 2022-2023
Funding Institute: Comunidad de Madrid
B. Limones

Programme: Programme I Investigate
Period: 2022-2023
Funding Institute: Comunidad de Madrid
P. Paramio

Programme: Programme I Investigate
Period: 2022 - 2023
Funding Institute: Comunidad de Madrid
R. Tomey

Programme: Programme I Investigate
Period: 2022 - 2023
Funding Institute: Comunidad de Madrid
L. Echevarría

Programme: Programme I Investigate
Period: 2022 - 2023
Funding Institute: Comunidad de Madrid
D. Rey

Programme: Programme I Investigate
Period: 2022 - 2023
Funding Institute: Comunidad de Madrid
J. Martínez

3. Scientific results

3.1. Publications

1. Barrejón M., Zummo F., Mikhalchan A., Vilatela J.J., Fontanini M., Scaini D., Ballerini L., Prato M. *TEGylated Double-Walled Carbon Nanotubes as Platforms to Engineer Neuronal Networks.* **ACS APPLIED MATERIALS AND INTERFACES,** 2022.
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12. Wang M., Yin G.-Z., Yang Y., Fu W., Díaz Palencia J.L., Zhao J., Wang N., Jiang Y., Wang D.-Y. *Bio-based flame retardants to polymers: A review.* **ADVANCED INDUSTRIAL AND ENGINEERING POLYMER RESEARCH,** 2022.
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Vilatela J. *Thermoconformable, Flexible Lithium-Ion Batteries.* **ADVANCED MATERIALS TECHNOLOGIES 7**, 2101635, 2022.

14. Yusuf A., Wang D.-Y. *Toward an In-Depth Fire Hazard and Resistance Diagnosis of Flame Retarded Liquid Electrolytes for Safer Lithium-Ion Batteries.* **ADVANCED MATERIALS TECHNOLOGIES 7**, 2101055, 2022.
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3.2. Book chapters

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2. T. Meštrović, J. Patterson. *Human Microbiome and Disease - chapter in Encyclopedia of Infection and Immunity*. In **Elsevier,** 662-673, 2022.
3. P. Alvaredo, J.M. Torralba, A. García-Junceda. *Sintering of High Entropy Alloys: Processing and Properties*. In **El Servier,** 362-371, 2022.
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3.3. Patent applications

1. *Nanowires network*. IMDEA Materials Institute. Patent application number EP21382408.9 (6 May 2021)
2. *A seismic detection system*. IMDEA Materials Institute and the Technical University of Madrid. Patent application number P202131218 (28 December 2021)

3.4. International conferences. Invited and plenary talks

1. *"New Instrumentation and Analysis Methodology for Nano-impact Testing"*, J.M. Molina-Aldareguia, **TMS 2022 Annual Meeting & Exhibition**, Anaheim, USA, February 2022.
2. *"Ciencia de datos para el descubrimiento y aplicación de nuevos materiales"*, M.Haranczyk, **FotoArt Workshop**, Madrid, Spain, March 2022.

3. *"The effect of elastic strains in the catalytic properties of transition metals"*, C. Martínez-Alonso, J. M. Guevara-Vela, J. LLorca, **18th European Mechanics of Materials Conference**, Oxford, UK, April 2022.
4. *"Design of Al alloys for additive manufacturing"*, C.M. Cepeda-Jiménez, C. Galera, M. San Sebastián, E. Gil, S. Milenkovic, J. LLorca, M.T. Pérez-Prado, **1st International Metal Additive Manufacturing Symposium**, Senlis, France, April 2022.
5. *"FFT based numerical study of elastic wave propagation in polycrystals"*, J. Segurado, R. Lebensohh, V. Rey-De-Pedraza, R. Sancho, P. Lafourcade, **EMMC18 / 18th European Mechanics of Materials Conference**, Oxford, UK, April 2022.
6. *"Progress on CNT fibre materials and applications"*, J.J. Vilatela, **The Carbon Hub Annual Technical meeting**, Houston, USA, May 2022.
7. *"Size effects in the deformation and fracture of nanolaminates"*, J.M. Molina-Aldareguia, **Congreso de la Sociedad Española de Cerámica y Vidrio**, Madrid, Spain, May 2022.
8. *"Micro y Nanomecánica: cuando el tamaño importa"*, J.M. Molina-Aldareguia, **II Ciclo de conferencias SOCIEMAT**, Madrid (Online), Spain, May 2022.
9. *"Microstructural design by additive manufacturing"*, M.T. Pérez-Prado, **Symposium "Additive Manufacturing the Future"**, Abu Dhabi, United Arab Emirates, May 2022.
10. *"Formation of grain boundaries during polycrystalline solidification of hcp alloys"*, A. Kaci Boukellal, M. Sarebanzadeh, A. Orozco-Caballero, J. LLorca, D. Tourret, **ICASP-6 / 6th International Conference on Advances in Solidification Processes**, Nancy, France, June 2022.
11. *"Modeling of Microstructures in Additive Manufacturing of Metals"*, D. Tourret, **Jornada de Fabricacion Aditiva MATERPLAT-READI**, Madrid, Spain, June 2022.
12. *"In situ synchrotron characterization of the mechanical and degradation behavior of WE43 Mg scaffolds for biomedical applications "*, J.M. Molina-Aldareguia, D. Martín-Alonso, F. Sket, G. Domínguez, M. Echeverry-Rendón, F. Benn, A. Kopp, J. LLorca, **ESMMC 2022. The European Solid Mechanics Conference**, Galway, Ireland, July 2022.
13. *"Additive manufacturing of multimaterial bioabsorbable polymer-metal devices including metallic particles or wires"*, C. Thompson, W. Ali, C. Pascual-González, M. Li, G. Domínguez, M. Echeverry-Rendón, C. González, J. LLorca, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.
14. *"In situ synchrotron characterization of the mechanical and degradation behavior of WE43 Mg scaffolds for biomedical applications"*, D. Martín-Alonso, F. Sket, G. Domínguez, M. Li, M. Echeverry-Rendón, F. Benn, A. Kopp, J. LLorca, J.M. Molina-Aldareguia, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.
15. *"A multiscale modelling roadmap for virtual design of precipitation-hardened metallic alloys"*, J. LLorca, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.

16. *"Multimaterial bioresorbable scaffolds manufactured by 3D printing for biomedical applications"*, J. LLorca, **Royal College of Surgeons in Ireland**, Dublin, Ireland, July 2022.
17. *"In situ synchrotron characterization of the mechanical and degradation behavior of WE43 Mg scaffolds for biomedical applications"*, J.M. Molina-Aldareguia, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.
18. *"An FFT framework for simulating non-local ductile failure"*, J. Segurado, **11th European Solid Mechanics Conference (ESMC 2022)**, Galway, Ireland, July 2022.
19. *"El futuro de la ciencia y los científicos en la sociedad española"*, J.M.Torralba, **Universidad Complutense-El Escorial**, El Escorial, Spain, July 2022.
20. *"Multiscale modelling strategy for metallic alloy selective laser melting"*, S. Mohammad Elahi, R. Tavakoli, A. Kaci Boukellal, T. Isensee, I. Romero, D. Tourret, **11th European Solid Mechanics Conference (ESMC)**, Galway, Ireland, July 2022.
21. *"Simulation of precipitation in Al-Li alloys"*, W. Shao, S. Liu J. LLorca, **PRISMS Center Annual Workshop**, Virtual, Virtual, August 2022.
22. *"Design of Al alloys for additive manufacturing"*, C.M. Cepeda-Jiménez, C. Galera, M. San Sebastián, E. Gil, S. Milenkovic, J. LLorca, M.T. Pérez-Prado, **9th World Congress on Particle Technology**, Madrid, Spain, September 2022.
23. *"Fracture behavior of metal-ceramic and metal-metal nanolaminates"*, J.M. Molina-Aldareguia, **10th International Workshop on Interfaces Design and Performance**, Santiago de Compostela, Spain, September 2022.
24. *"Additive manufacturing of smart alloys for biodegradable and smart implants"*, J.M. Molina-Aldareguia, **Biomedical and bioinspired materials and structures: a cross-disciplinary approach**, Vienna, Austria, September 2022.
25. *"Additive manufacturing of advanced alloys for biodegradable and smart implants"*, J.M. Molina-Aldareguia, L. Martín-Alonso, F. Sket, M. Li, M. Echeverry-Rendón, A. Kopp, J. LLorca, **KMM-VIN / ViCEM / ESB cross-disciplinary workshop on biomedical and bioinspired materials and structures: a cross-disciplinary approach**, Vienna, Austria, September 2022.
26. *"FFT based numerical study of elastic wave propagation in heterogeneous media: application to polycrystals"*, J. Segurado, R. Lebensohn, V. Rey-De-Pedraza, R. Sancho, P. Lafourcade, **SES Meeting 2022**, College Station, TX, USA, September 2022.
27. *"Adaptive grids for FFT based Field Dislocation Mechanics and KMC simulations"*, J. Segurado, R. Lebensohn, V. Rey-De-Pedraza, R. Sancho, P. Lafourcade, **SES Meeting 2022**, College Station, TX, USA, September 2022.
28. *"FFT based numerical study of elastic wave propagation in heterogeneous media: application to polycrystals"*, J. Segurado, R. Lebensohn, V. Rey-De-Pedraza, R. Sancho, P. Lafourcade, **24th International Conference on Computer Methods in Mechanics (CMM) and the 42nd Solid Mechanics Conference (SolMech)**, Świnoujście, Poland, September 2022.
29. *"Impresión 3D y sostenibilidad"*, M.T. Pérez-Prado, **Jornada de Sociedades COSCE 2022**, Madrid, Spain, September 2022.

30. *“Multiscale modelling and in situ characterization strategies at IMDEA Materials Institute: roadmaps for virtual processing and virtual testing of metallic alloys”*, J. LLorca, D. Tourret, J. Segurado, I. Romero, J.M. Molina-Aldareguia, F. Sket, **10th International Conference on Multiscale Materials Modeling**, Baltimore, Maryland, USA, October 2022.
31. *“Multiscale Modeling of Dendritic Growth with Fluid Flow”*, D. Tourret, T. Isensee, **International Conference on Multiscale Materials Modeling (MMM10)**, Baltimore, USA, October 2022.
32. *“Topological gallery of non-Hermitian whispers”*, J. Christensen, **2022 International Ultrasonic Symposium**, Venice, Italy, October 2022.
33. *“PM Production Routes”*, J.M. Torralba, M. Campos, P. Alvaredo, A. García Junceda, A. Meza, S. Venkatesh Kumaran, A. Mohammadzadeh, **World PM2022 Congress & Exhibition (at the Young Engineers Day)**, Lyon, France, October 2022.
34. *“High Entropy Alloys: An Opportunity for the PM route”*, J.M. Torralba, Mónica Campos, P. Alvaredo, A. García Junceda, A. Meza, S. Venkatesh Kumaran, A. Mohammadzadeh, **World PM2022 Congress & Exhibition (At Special Interest Seminar on High Entropy Alloys)**, Lyon, France, October 2022.
35. *“Multiscale modelling and in situ characterization strategies at IMDEA Materials Institute: roadmaps for virtual processing and virtual testing of metallic alloys “*, J. LLorca, D. Tourret, J. Segurado, I. Romero, J.M. Molina-Aldareguia, F. Sket, **MMM10 -The 10th International Conference on Multiscale Materials Modeling**, Baltimore, USA, October 2022.
36. *“Modeling of microstructure formation and evolution in advanced manufacturing of metals”*, D. Tourret, **ICAMS Advanced Discussions on “Advanced models for microstructure evolution – process-microstructure-property relationships”**, Bochum, Germany, October 2022.
37. *“On the effect of 3D grain boundary orientation on slip transfer”*, E. Nieto-Valeiras, E. Ganju, N. Chawla, J. LLorca, **MRS Fall meeting**, Boston, Massachusetts, USA, November 2022.
38. *“Additive manufacturing of energy saving materials”*, M.T. Pérez-Prado, **Open Innovation and Industrial workshop, iMPLANTS-CM (Technical University of Madrid)**, Madrid, Spain, November 2022.
39. *“Trends in organ-on-chip devices and in vitro tissue models”*, J. Patterson, **iMPLANTS-CM Open-Innovation Workshop**, Madrid, Spain, November 2022.
40. *“Topological sound and vibrations”*, J. Christensen, **Nano seminars series, ICN2**, Barcelona, Spain, December 2022.

3.5. International conferences. Regular contributions

1. *“Multiscale modeling of Ni alloys laser powder-bed fusion”*, S. Mohammad Elahi, R. Tavakoli, A. Kaci Boukellal, T. Isensee, I. Romero, D. Tourret, **TMS Annual Meeting**, California, USA, February-March 2022.

2. *"Multiscale dendritic needle network study of the effect of buoyant liquid flow on dendritic growth kinetics"*, T. Isensee, D. Tourret, **TMS Annual Meeting**, California, USA, February-March 2022.
3. *"Modeling of phase transformation kinetics in Ti6Al4V alloy during additive manufacturing"*, A. Boccardo, X. Yang, D. Tourret, J. Segurado, Z. Zou, M. Simonelli, M. Tong, S. Leen, **TMS Annual Meeting**, California, USA, February-March 2022.
4. *"In situ synchrotron characterization of the fatigue behavior of WE43 Mg porous scaffolds for biomedical applications"*, J.M. Molina-Aldareguia, **TMS Annual Meeting**, California, USA, February-March 2022.
5. *"Role of misorientation on grain boundary sliding through high resolution digital image correlation"*, A. Orozco-Caballero, E. Nieto-Valeiras, J. LLorca, F. Carreño, **TMS Annual Meeting**, California, USA, February-March 2022.
6. *"Development and 3D Printing of a bioabsorbable composite material for orthopaedic applications"*, C. Thompson, C. Pascual-González. G. Domínguez, M. Echeverry-Rendón, C. González, J. LLorca, **TMS 2022**, California, USA, February-March 2022.
7. *"Slip transfer and cracking at grain boundaries in FCC and HCP metals"*, E. Nieto-Valeiras, M. Sarebanzadeh, M. Zhang, A. Orozco-Caballero, J. LLorca, F. Carreño, **TMS Annual Meeting 2022**, California, USA, February-March 2022.
8. *"In situ synchrotron characterization of the fatigue behavior of WE43 Mg porous scaffolds for biomedical applications"*, D. Martín, G. Domínguez, M. Li, F. Sket, M. Echeverry-Rendón, F. Benn, A. Kopp, J.M. Molina-Aldareguia, J. LLorca, **TMS Annual Meeting**, California, USA, March 2022.
9. *"Formation of grain boundaries during polycrystalline solidification of hcp alloys"*, A.K. Boukellal, M. Sarebanzadeh, A. Orozco-Caballero, F. Sket, J. LLorca, D. Tourret, **TMS Annual**, California, USA, March 2022.
10. *"Laminated structural power composites produced with mechanically-connected electric double-layer capacitors"*, C. González, Y. Ou, M. Rana, J.J. Vilatela, **18th European Mechanics of Materials Conference (EMMC18)**, Oxford, UK, April 2022.
11. *"Multiscale modeling of Ni alloys laser powder-bed fusion"*, S. Mohammad Elahi, R. Tavakoli, A. Kaci Boukellal, T. Isensee, I. Romero, D. Tourret, **18th European Mechanics of Materials Conference (EMMC18)**, Oxford, UK, April 2022.
12. *"Study of the effect of strain rate on the in-plane shear and transverse compression response of a composite ply using computational micromechanics"*, M. Rueada Ruiz, M. Herráez, F. Sket, C. González, J.M. Molina-Aldareguia, **18th European Mechanics of Materials Conference (EMMC18)**, Oxford, UK, April 2022.
13. *"First principles prediction of Al-Cu, Al-Li and Al-Cu-Li phase diagrams"*, S. Liu, J. LLorca, **18th European Mechanics of Materials Conference (EMMC18)**, Oxford, UK, April 2022.
14. *"Optimization of the SLM processing parameters of the Inconel 939"*, I. Rodríguez-Barber, A.M. Fernández-Blanco, I. Unanue-Arruti, I. Madariaga-Rodríguez, S. Milenkovic, M.T. Pérez-Prado, **18th European Mechanics of Materials Conference (EMMC18)**, Oxford, UK, April 2022.

15. *"Slip transfer mechanisms at grain boundaries in FCC and HCP metals"*, M. Sarebanzadeh, E. Nieto-Valeiras, I. Escobar-Moreno, A. Orozo-Caballero, J. LLorca, **18th European Mechanics of Materials Conference (EMMC18)**, Oxford, UK, April 2022.
16. *"Fatigue crack initiation mechanisms in Mg alloys: effect of grain size and grain boundary misorientation"*, S. Jamali, A. Ma, J. LLorca, **18th European Mechanics of Materials Conference (EMMC18)**, Oxford, UK, April 2022.
17. *"Control of strain hardening ability and uniform elongation via microstructural design in martensitic stainless steels."*, A. Sierra-Soraluce, G. Li, I. Sabirov, J.M. Molina-Aldareguia, M.J. Santofimia, A. Smith, **25th International Conference on Material Forming - ESAFORM 2022**, Braga, Portugal, April 2022.
18. *"First principles prediction of Al-Cu, Al-Li and Al-Cu-Li phase diagrams". "*, S. Liu, W. Shao, J. LLorca, **6th World Congress on Integrated Computational Materials Engineering (ICME 2022)**, Lake Tahoe, Nevada, USA, April 2022.
19. *"Suspended 1D nanomaterials: synthesis via floating catalyst and direct assembly as high-performance network materials "*, J.J. Vilatela, **Nanowire Week**, Chamonix, France, April 2022.
20. *"Benchmark simulations of multiscale models for dendritic growth in alloys under isothermal and directional conditions"*, T. Isensee, D. Tourret, A. Viardin, L. Sturz, M. Založnik, **6th International Conference on Advances in Solidification Processes (ICASP-6)**, Nancy, France, June 2022.
21. *"A Bayesian approach for cohesive parameters inference in translaminar fracture",* C. González**, XIV National Congress on Composite Materials**, Sevilla, Spain, June 2022.
22. *"Relación entre la microestructura-topología y propiedades mecánicas de andamios basados en Mg impresos en 3D para aplicaciones biomédicas"*, M.D. Martin-Alonso, G. Domínguez, M. Li, M. Echeverry-Rendón, F. Benn, A. Kopp, J. LLorca, J.M. Molina-Aldareguia, F. Sket, **CNMAT - XVI Congreso Nacional de Materiales**, Ciudad Real, Spain, June 2022.
23. *"Thermomechanical calibration of constitutive material models for ballistic impact simulation"*, J.L. de Pablos, I. Romero, **International Forum on Aeroelasticity and Structural Dynamics (IFASD 2022)**, Madrid, Spain, June 2022.
24. *"High-cycle fatigue behavior of quenching and partitioning (Q&P) treated stainless steels"*, A. Sierra-Soraluce, J.M. Molina-Aldareguia, A. Smith, M. Muratori, I. Sabirov, **19th International Conference on Strength of Materials – ICSMA19**, Metz, France, June 2022.
25. *"Helical phyllotaxis and conventional laboratory diffraction contrast tomography (LabDCT) acquisition strategies for characterization of 3D grain orientations"*, E. Ganju, E. Nieto-Valeiras, J. LLorca, N. Chawla, **6th International Congress on 3D Materials Science (3DMS 2022)**, Washington DC, USA, June 2022.
26. *"Manufacturing, mechanical and degradation behavior of Mg/PLA bioresorbable composite laminates for orthopedic applications"*, W. Ali, L. Tillmann A. Kopp, C. González, J. LLorca, **20th European Conference on Composite Materials (ECCM20)**, Lausanne, Switzerland, June 2022.

27. *“Assessing porosity morphology in composite materials by analysis of frequency response”*, J.I. Caballero-Garzon, G. Cosarinsky, J. Camacho, E. Menasalvas, C. Gonzalo-Martin, F. Sket, C. González, **20th European Conference on Composite Materials (ECCM20)**, Lausanne, Switzerland, June 2022.
28. *“Helical phyllotaxis and conventional laboratory diffraction contrast tomography (LabDCT) acquisition strategies for characterization of 3D grain orientations”*, E. Ganju, E. Nieto, J. LLorca, N. Chawla, **6th International Congress on 3D Materials Science (3DMS 2022)**, Washington DC, USA, June 2022.
29. *“High entropy alloys MnCrFe2Ni2 produced by selective laser melting”*, R. Castellote-Alvarez, I. Toda-Caraballo, C. Fernández-Jiménez, J. García-Arisco, S. Milenkovic, J.M. Molina-Alderaguia, D. San-Martín, **Congreso Nacional de Materiales (CNMAT)**, Ciudad Real, Spain, June-July 2022.
30. *“Additive manufacturing of the nickel-based superalloy Inconel 939: correlation between processing parameters, defectology and microstructure”*, I. Rodríguez-Barber, A.M. Fernández-Blanco, I. Unanue-Arruti, I. Madariaga-Rodríguez, S. Milenkovic, M.T. Pérez-Prado, **Congreso Nacional de Materiales (CNMAT)**, Ciudad Real, Spain, June-July 2022.
31. *“Design and development of high entropy CoNi based superalloy: CALPHAD method and metallurgical assessments”*, A. Mohammadzadeh, J.M. Torralba, **Congreso Nacional de Materiales (CNMAT)**, Ciudad Real, Spain, June-July 2022.
32. *“Diseño de nuevas superaleaciones ligeras base cobalto sinterizadas”*, A. Mejia-Reinoso, S. Hong, L.A. Díaz Rodríguez, J.M. Torralba, M. Campos, **Congreso Nacional de Materiales (CNMAT)**, Ciudad Real, Spain, June-July 2022.
33. *“Developing competitive high entropy alloys by spark plasma sintering using commercial commodity powders”*, S.V. Kumaran, D. Garbiec, J.M. Torralba, **Congreso Nacional de Materiales (CNMAT)**, Ciudad Real, Spain, June-July 2022.
34. *“Efectos de la exposición a alta temperatura de aceros martensíticos formadores de alúmina para generación de energía”*, F. Masari, J.M. Torralba, L. Díaz Rodríguez, M. Campos, **Congreso Nacional de Materiales (CNMAT)**, Ciudad Real, Spain, June-July 2022.
35. *“A cost-effective and energy-efficient way to develop competitive high entropy alloys by powder metallurgy”*, S.V. Kumaran, D. Garbiec, J.M. Torralba, **16th International Conference on Nanostructured Materials (NANO2022)**, Seville, Spain, June-July 2022.
36. *“Alumina-forming martensitic alloys for application in high-temperature energy generation systems”*, F. Masari, J.M. Torralba, L. Díaz Rodríguez, M. Campos, **16th International Conference on Nanostructured Materials (NANO2022)**, Seville, Spain, June-July 2022.
37. *“Development of a new low-density sintered superalloys based on Co* $\alpha\alpha'$», M. Reinoso A, S. Hong, L. Díaz Rodríguez, J.M. Torralba, M.C. Gómez, **16th International Conference on Nanostructured Materials (NANO2022)**, Seville, Spain, June-July 2022.
38. *“Physical and thermodynamic simulation of functionally graded materials”*, J. Valilla Robles, D. Tourret, I. Sabirov, **Junior EUROMAT 2022**, Coimbra, Portugal, July 2022.

39. *“Cu-Mn cosegregation in MnCrFe2Ni2 base HEAs produced by different manufacturing routes”*, R. Castellote-Alvarez, I. Toda-Caraballo, C. Fernández-Jiménez, J. García-Arisco, S. Milenkovic, J.M. Molina-Alderaguia, D. San-Martín, **Junior EUROMAT 2022**, Coimbra, Portugal, July 2022.
40. *“A FS-GPU implementation to increase the computational performance of phase-dield model resolution”*, A. Boccardo, J. Segurado, M. Tong, S. Leen, D. Tourret, **Junior EUROMAT 2022**, Coimbra, Portugal, July 2022.
41. *“Fatigue crack initiation and propagation mechanisms in quenching and partitioning (Q&P) treated stainless steels. “*, A. Sierra-Soraluce, J.M. Molina-Aldareguia, A. Smith, M. Muratori, I. Sabirov, **Junior EUROMAT**, Coimbra, Portugal, July 2022.
42. *“Effect of interfacial segregation on the interaction between dislocations and precipitates in Mg alloys”*, X.Z. Jin, S. Milenkovic, I. Sabirov, M.T. Pérez-Prado, **International Conference on Strength of Materials**, Metz, France, July 2022.
43. *“A mechanician’s journey towards understanding non-equilibrium thermodynamics”*, I. Romero, **ICMAT**, Madrid, Spain, July 2022.
44. *“Eliminating solvents and polymers in high-performance Si anodes by gas phase assembly of nanowire fabrics”*, J.J. Vilatela, **Power our Future**, Vitoria, Spain, July 2022.
45. *“Multiscale modelling strategy for metallic alloy selective laser melting”*, D. Tourret, R. Tavakoli, M. Elahi, A.K. Boukellal, T. Isensee, I. Romero, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.
46. *“Thermoelastic metamaterials with shape memory”*, I. Romero, A. Vasudevan, J. A. Rodríguez-Martínez, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.
47. *“Manufacturing, mechanical behavior and biocompatibility of PLA/Mg fibers laminates for orthopedic applications”*, W. Ali, L. Tilmann, G. Domínguez, M. Echeverry-Rendón, A. Kopp, C. González, J. LLorca, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.
48. *“Additive manufacturing of bioabsorbable polymer/metal particle (Mg or Zn) composites for orthopaedic applications “*, C. Thompson, C. Pascual-González, M. Echeverry-Rendón, C. González, J. LLorca, **11th European Solid Mechanics Conference**, Galway, Ireland, July 2022.
49. *“Modeling of martensite decomposition in Ti6Al4V alloy during heat treatments after additive manufacturing processing”*, A. Boccardo, J. Segurado, Z. Zou, M. Simonelli, M. Tong, S. Leen, D. Tourret, **11th European Solid Mechanics Conference (ESMC)**, Galway, Ireland, July 2022.
50. *“Dragged solids: three-dimensional solids with the kinematics of geometrically exact models”*, I. Romero, R. Cantón-Sánchez, D. Portillo, **World Congress on Computational Mechanics WCCM-APCOM 2022**, Yokohama, Japan, July-August 2022.
51. *“3D printed Mg-based scaffolds for temporary bone replacement applications”*, M.D. Martín-Alonso, **Symposium on Biodegradable Metals**, Alicante, Spain, August, 2022.

52. *"Fatigue performance of quenching and partitioning (Q&P) treated martensitic stainless steels"*, A. Sierra-Soraluce, J.M. Molina-Aldareguia, A. Smith, M. Muratori, I. Sabirov, **10th International Conference on Fracture Fatigue and Wear (FFW 2022) (online),** Gent, Belgium, August 2022.
53. *"3D printed Mg-based scaffolds for temporary bone replacement applications"*, M.D. Martin-Alonso, G. Domínguez, M. Li, M. Echeverry-Rendón, F. Benn, A. Kopp, J. LLorca, J.M. Molina-Aldareguia, F. Sket, **BIOMETALS - 14th Symposium on Biodegradable Metals**, Alicante, Spain, August 2022.
54. *"Nonlinear preconditioning of phase-field based structural topology optimization problems"*, R. Tavakoli and D. Tourret, **11th International Conference on Engineering Computational Technology**, Montpellier, France, August 2022.
55. *"Theory and numerical methods for the simulation of nonlinear mechanics of dragged slender solids: the case of fat rods and shells"*, I. Romero, R. Cantón-Sánchez, D. Portillo, **Congreso de Métodos Numéricos en Ingeniería (CMN2022)**, Las Palmas de Gran Canarias, Spain, September 2022.
56. *"Mechanical properties and strain hardening behaviour of quenching and partitioning (Q&P) treated martensitic stainless steels"*, A. Sierra-Soraluce, G. Li, I. Sabirov, J.M. Molina-Aldareguia, M.J. Santofimia, M. Muratori, A. Smith, **MSE 2022 Congress**, Darmstadt, Germany, September 2022.
57. *"First principles predictions of the Al-Li phase diagram"*, W. Sha., S. Liu, J. LLorca, **18th Discussion Meeting on Thermodynamics of Alloys (TOFA2022)**, Krakow, Poland, September 2022.
58. *"Preparation of elastomeric polyurethane photo-curable resins for stereolithography 3D printing"*, P. Navarrete Segado, J.P. Fernández Blázquez, J.P., Á. Castro María, Á., Camacho, Á., Patterson, J., **European Society for Biomaterials Annual Meeting**, Bordeaux, France, September 2022.
59. *"Characterization of gelatin hydrogels for 3D bioprinting and tissue engineering"*, Á. Castro María, J.P. Fernández Blázquez, J. Patterson, **European Society for Biomaterials Annual Meeting**, Bordeaux, France, September 2022.
60. *"Pre-alloyed powders of Ti-Fe ultrafine eutectics for laser additive manufacturing"*, A.K Pandey, P. Alvaredo, S. Milenkovic, F, Sket, **9th World Congress on Particle Technology (WCPT9)**, Madrid, Spain, September 2022.
61. *"Thermal treatment study of L-PBFed IN939 superalloy"*, I. Rodríguez-Barber, A.M. Fernández-Blanco, I. Unanue-Arruti, I. Madariaga-Rodríguez, S. Milenkovic, M.T. Pérez-Prado, **Alloys for Additive Manufacturing Symposium**, Munich, Germany, September 2022.
62. *"Using mixes of prealloyed commodity powders to develop competitive high entropy alloys by selective laser melting"*, S.V. Kumaran, A. Meza, J. M. Torralba, **Alloys for Additive Manufacturing Symposium 2022 (AAMS22)**, Munich, Germany, September 2022.
63. *"Design of novel sintered W-Free Co-based alloys"*, A. Mejía-Reinoso, M. Campos, S. Hong, L.A. Díaz Rodríguez, J.M. Torralba, **World PM2022 Congress & Exhibition**, Lyon, France, October 2022.

64. *"Corrosion behaviour at high temperature of alumina-forming martensitic steels for energy generation systems"*, F. Masari, L.A. Díaz Rodríguez, J.M. Torralba, M. Campos, **World PM2022 Congress & Exhibition**, Lyon, France, October 2022.
65. *"Towards machine learning segmented porosity in ultrasonic tests for composite materials"*, J.I. Caballero-Garzon, G. Cosarinsky, J. Camacho, E. Menasalvas, C. Gonzalo-Martin, F. Sket, C. González, **NDE4.0**, Berlin, Germany, October 2022.
66. *"Impresión 4D Empleando Polímeros Y Aleaciones Con Memoria De Forma Para Una Nueva Generación De Dispositivos Médicos Inteligentes"*, J.M. Molina-Aldareguia, **XV Congreso Iberoamericano de Ingeniería Mecánica**, Madrid, Spain, November 2022.
67. *"First principles calculation of the phase diagrams of alloy of technological interest including configurational and vibrational entropic contributions"*, W. Shao, S. Liu, J. LLorca, **MRS Fall Meeting**, Boston, Massachusetts, USA, November 2022.
68. *"Effect of elastic strains on the catalytic activity of intermetallic compounds for the hydrogen economy"*, C. Martínez-Alonso, T. Xie, J. M. Guevara-Vela, K. T. Winther, F. Abild-Pedersen, J. LLorca, **MRS Fall Meeting**, Boston, Massachusetts, USA, November 2022.
69. *"Machine Learning-Aided Strategy to Discover Intermetallic Catalysts for the Hydrogen Evolution and the Oxygen Reduction Reactions"*, C. Martínez-Alonso, T. Xie, J. M. Guevara-Vela, K. T. Winther, F. Abild-Pedersen, J. LLorca, **MRS Fall Meeting**, Boston, Massachusetts, USA, November 2022.
70. *"New tendency of flame-retardant Li-battery "*, D.Y. Wang, **Fire Resistance in Plastics**, Cologne, Germany, November 2022.
71. *"The effect of microstructure on fatigue behaviour of a Fe-Mn-Al-C steel"*, A. Gómez Fernández, M. Avela, J.M. Molina-Aldareguia, A. Dutta, I. Sabirov, **8th International Conference of the Hellenic Metallurgical Society**, Patras, Greece, December 2022.
72. *"The effect of stress state on the microstructure evolution during plastic deformation of Q&P treated martensitic stainless steels"*, A. Sierra-Soraluce, J. L. De Pablos, J.M. Molina-Aldareguia, A. Smith, M. Muratori, I. Sabirov, **8th International Conference of the Hellenic Metallurgical Society**, Patras, Greece, December 2022.

3.6. International conferences. Membership in organising committees

1. **TMS Annual Meeting**. Dr. D. Tourret (Symposium Organiser *"Computational Thermodynamics & Kinetics"*). V. Attari, S. Kadkhodaei, E. Zarkadoula, D. Tourret, J. R. Morris, Anaheim, CA, USA, February-March, 2022.
2. **Society for Biomaterials Annual Meeting**. Dr. J. Patterson (Session Organizer). Baltimore, USA, April, 2022.
3. **Beamtime Allocation Panel of European Synchrotron Radiation facility for ID17, BM18 and ID19 beamlines**. Dr. F. Sket (e.g. BAP member). Online / Grenoble, France, April, 2022.

4. **European Mechanics of Materials Conference (EMMC18).** Dr. M.T. Pérez-Prado (Symposium Organiser *"Additive manufacturing and related materials processing").* Oxford, UK, April, 2022.
5. **International Conference on the Science of nanotubes and low dimensional materials.** Dr. M.T. Pérez-Prado (Symposium Organiser). J.J. Vilatela, Swon, Korea, June.
6. **ICASP-6 / 6th International Conference on Advances in Solidification Processes**. Dr. D. Tourret (Scientific Board member). Nancy, France, June, 2022.
7. José Vilatela (Symposium Organiser). Swon, Korea, June, 2022.
8. **ICSMA 2022: The 19th International Conference on Strength of Materials.** Dr. M.T. Pérez-Prado (International Advisory Board Member). Metz, France, June-July, 2022.
9. **16th International Conference on Nanostructured Materials NANO2022**. Prof. J.M. Torralba (Symposium Organizer). Seville, Spain, June-July, 2022.
10. **Experimental Micro and Nanomechanics - 11th European Solid Mechanics Conference**. Dr. J.M. Molina-Aldareguia (Symposium organizer). J.M. Molina-Aldareguia / G. Dehm / M. Monclús, Galway, Ireland, July, 2022.
11. **European Solid Mechanics Conference.** Prof. I. Romero (Symposium organizer). Galway, Ireland, July, 2022.
12. **CSIC/IMDEA**. Prof. I. Romero (Co-chairman). Madrid, Spain, July.
13. **World Congress on Computational Mechanics WCCM-APCOM 2022**. Prof. I. Romero (Symposium organizer). Yokohama, Japan, July-August, 2022.
14. **International Conference on the Science of nanotubes and low dimensional materials**. Dr. Juan
15. **AAMS22, Alloys for additive manufacturing symposium 2022**. Dr. M.T. Pérez-Prado (Scientific Committee member). Munich, Germany, September, 2022.
16. **WCPT9, 9th World Congress on Particle Technology**. Dr. M.T. Pérez-Prado (Scientific Committee member). Madrid, Spain, September, 2022.
17. **MSE Congress 2022**. Dr. I. Sabirov (International Congress). P.E. Di Nunzio, U. Krupp, U. Prahl, A. Smith, I. Sabirov, Darmstadt, Germany, September, 2022.
18. **International Conference on Multiscale Materials Modeling (MMM10)**. Dr. D. Tourret (Symposium Organizer *"Interface-driven Phenomena in Condensed Matter Systems: Thermodynamics, Kinetics, and Chemistry"*). F. Abdeljawad, H. Fan, Y. Shibuta, T. Suzudo, M. Taheri, D. Tourret, M. Zaiser, USA, October, 2022.
19. **Biomedical Engineering Society Annual Meeting**. Dr. J. Patterson (Abstract Reviewer). San Antonio, USA, October, 2022.
20. **Society of Women Engineers Annual Meeting**. Dr. J. Patterson (Abstract Reviewer). Houston, USA, October, 2022.
21. **World PM2022 Congress & Exhibition**. Prof. J.M Torralba (Steering Committee). Lyon, France, October, 2022.
22. **World PM2022 Congress & Exhibition**. Prof. J.M. Torralba (Co-chairmen of the Technical Programme). Lyon, France, October, 2022.
23. **ISFRMT2022**. Dr. D-Y Wang (member of international scientific committee), Beijing, China, November, 2022.

24. **Congreso Iberoamericano de Ingeniería Mecánica.** Prof. I. Romero (Local organising committee). Madrid, Spain, November.

3.7. Invited seminars and lectures

1. "*Microstructure selection during solidification processes: Insight from multiscale modeling approaches*", D. Tourret, **Sharif University**, Tehran, Iran (online), March, 2022
2. *"Microstructure selection in solidification processes: Insight from multiscale modeling",* D. Tourret, **National University of Ireland**, Galway, Ireland, July, 2022
3. *"Bayesian calibration of complex models. Application to elasto-plastic constitutive relations"*, I. Romero, **Universidad de Zaragoza**, Zaragoza, Spain, April, 2022
4. *"Variational formulations for the solution of coupled and structural problems"*, I. Romero, **Ansys, Inc., Canonsburg**, U.S., July, 2022
5. *"Mg scaffolds manufactured by power bed laser fusion for orthropaedic applications",* D. Martín-Alonso, G. Domínguez, M. Li, F. Sket, M. Echeverry, F. Benn, A. Kopp, J.M. Molina-Aldareguia, J. LLorca, Department of Mechanical and Aerospace Engineering, **Nanyang Technological University**, Singapore, February, 2022
6. *"A roadmap for virtual design of precipitation-hardened metallic alloys: application to Al-Cu"*, J. LLorca, **Institute for High Performance Computing, Agency for Science, Technology and Research**, Singapore, February, 2022
7. "*Effect of elastic strains on the catalytic properties of transition metals and intermetallic compounds"*, C. Martínez-Alonso, T. Xie, J. M. Guevara-Vela, J. LLorca, SUNCAT, **Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory**, Menlo Park, California, USA, March, 2022
8. *"Mg scaffolds manufactured by power bed laser fusion for orthopedic applications",* D. Martín-Alonso, G. Domínguez, M. Li, F. Sket, M. Echeverry-Rendón, F. Benn, A. Kopp, J.M. Molina-Aldareguia, J. LLorca, **Imperial College**, London, UK, April, 2022
9. *"3D printed multimaterial bioabsorbable scaffolds for bone tissue engineering: mechanical, corrosion and biological performance"*, J. LLorca, Department of Solid Mechanics, **KTH Royal Institute of Technology**, Sweden, November, 2022
10. *"An FFT framework for simulating non-local ductile failure",* J. Segurado, **Los Alamos NL**, Los Alamos, USA, July, 2022
11. *"FFT based computational homogenization",* J. Segurado, **Texas A&M** in CSM3 summer course, College station, USA, July, 2022
12. *"Nanoindentation at impact rates",* J.M. Molina-Aldareguia, **Surface Ventures**, Online, United Kingdom, February, 2022
13. *"High Temperature Materials",* J.M. Torralba, **EPMA Summer School**, Ciudad Real, Spain, June, 2022
14. *"The Battery Show",* J.J. Vilatela, **The Battery Show**, Stuttgart, Germany, June, 2022
15. *"Panel Sustainable Future Through Advanced Materials",* J.J. Vilatela, **Puzzle X**, Barcelona, Spain, November, 2022

16. *"Nanotextile electrodes produced by gas phase assembly",* J.J. Vilatela, **Münster University**, Münster, Germany, December, 2022
17. *"Suspended 1D nanomaterials: synthesis via floating catalyst and direct assembly as high-performance network materials ",* J.J. Vilatela, **Rensselaer Polytechnic Institute**, Troy, US, April, 2022
18. *"Additive manufacturing of energy-saving materials",* M.T. Pérez-Prado, **Sharif University of Technology**, Sharif, Iran, December, 2022
19. *"Microstructural design by additive manufacturing",* M.T. Pérez-Prado, **University of Oxford**, Oxford, UK, November, 2022

3.8. Awards

1. Ph.D. with Distinction (premio extraordinario de doctorado), Technical University of Madrid, 2022, **Y. Ou.**
2. 2021 Acta & Scripta Materialia Outstanding Reviewer Award, 2022, **D. Tourret.**
3. The best oral presentation award at the 10th International Conference on Fracture Fatigue and Wear 2022, International Conference on Fracture Fatigue and Wear (University of Ghent), August 2017, **A. Sierra-Soraluce.**
4. Acta Materialia Student Award, Acta Journals Inc., 2022, **B. Bellón.**
5. Outstanding Reviewer Award 2022 for the journals Biofabricatoin and Journal of Physics: Materials, IOP (publisher), 2022, **J. Patterson.**
6. Ivor Jenkins Gold Medal, Institute of Materials, Minerals & Mining, 2022, **J.M.Torralba.**

3.9. Seminars

1. "*All-Electrochemical Graphene Composite Multilayers Deposited on Carbon Fibers and 3D-Foams for Energy Storage"*, Dr. Jaime S. Sanchez (from the University of Technology, Sweden). January 2022.
2. *"Modeling advanced materials across length scales: toward an application-specific computational design"*, Dr. Javad Kadkhodapour (from Stuttgart University, Germany). January 2022.
3. *"Alloy plasticity: insights from ab initio and elasticity"*, Dr. David Rodney (from the University of Lyon, France). February 2022.
4. *"Elasto-plastic stochasticity: the role of atomic level fluctuations on mesoscale deformation properties in metals"*, Prof. Jaime Marian (from UCLA and visiting researcher at IMDEA Materials Institute). February 2022.
5. *"Computational design of ultra-strong high-entropy alloys manufactured via additive manufacturing processes"*, Dr. Mauricio Ponga (from the University of British Columbia, Canada). May 2022.

6. *"3D shaping of carbon to engineered living carbon materials"*, Dr. Monsur Islam (from the Institute for Microstructure Technology, Karlsruhe Institute of Technology, Germany). May 2022
7. *"Engineering Materials for the Translation of Biomedical Devices",* Dr. Kendell Pawelec (from Michigan State University, USA). June 2022.
8. *""Towards 3D+ Printing of Metals and Alloys"*, Dr. Raymundo Arróyave (from Texas A&M University, USA). June 2022.
9. *Residual stresses and hydrogen embrittlement"*, Prof. Jesús Ruiz (from the Technical University of Madrid, Spain). July 2022.
10. *"Lactate as a novel signal for cardiac tissue engineering and regenerative medicine",* Dr. Jesús Ordoño (from the Institute for Health Science Research Germans Trias i Pujol (IGTP), Spain). July 2022.
11. *"Lightweight materials and sustainable manufacturing: the role of ICME"*, Alan Luo (from Ohio State University, USA, and Director of the "Lightweight Materials and Manufacturing Research Lab"). September 2022.
12. *"Research and development activities in Nano4Energy: from laboratory-scale development of thin films to industrial production"*, Ivan Fernández (from Nano4Energy SL., Spain). September 2022.
13. *"Simulating Plasticity in Metals at Atomistic and Mesoscopic Length Scales"*, Douglas E. Spearot (from the University of Florida, USA and current visitor at IMDEA Materials). September 2022.
14. *"Dynamic plastic localization and fragmentation of porous printed metals: impact experiments and multiscale modeling"*, Prof. Jose A. Rodríguez-Martínez (from the University Carlos III of Madrid, Spain). October 2022.
15. *"Deformation mechanisms in metals – Insights from molecular dynamics simulations"*, Dr. Carlos Ruestes (from IMDEA Materials Insitute, Spain - Marie Skłodowska–Curie Actions Postdoctoral Fellow). November 2022.
16. *"Form Follow Function vs Function Follows form: a shift in tissue regeneration"*, Dr. Sandra Camarero (from the POLYMAT Institute, Spain). December 2022.

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 online 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: Seismic detection system
Description: Sensor device that allows the detection of seismic waves and plenty of physical magnitudes characteristic of them, through a wide range of frequencies, capable of communicating data signals in real time. The device is also mechanically robust and capable to withstand extreme environmental conditions.
Opportunity: Technology License

Title: High-porosity composite phase-change materials for thermal energy storage applications
Description: Shape-stabilised composite phase-change material (PCM), physically stable and with high phase change enthalpy. The material is suitable for thermal management applications in electronics, power electronics, solar energy, batteries, or construction.
Opportunity: Technology License

Title: Recyclable and curved sandwich composites through bendable benzoxazine-based foaming core
Description: Vitrimer-based syntactic foams with application in recyclable and curved lightweight sandwich composites manufactured by hot-press, for flexible interiors in the transportation, aerospace and defense industries, as well as in construction.
Opportunity: Technology License

Title: Smart mask that monitors breath rhythm
Description: Smart face mask with self-powered sensors capable of monitoring vital parameters such as respiration rate and characteristics of respiration pulses that wirelessly transmits them through IoT protocols to a telemedicine platform.
Opportunity: Technology License

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: Electrode for capacititive deionisation
Description: Electrode for capacitive deionisation in which the active phase and the current collector are included in a single element, i.e. a composite material.
Opportunity: Technology License

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

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

Title: FFTMAD (Fast Fourier Transform Based Homogenisation Code, MADrid)
Description: FFT-based simulation tool developed by IMDEA Materials for computational homogenisation 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

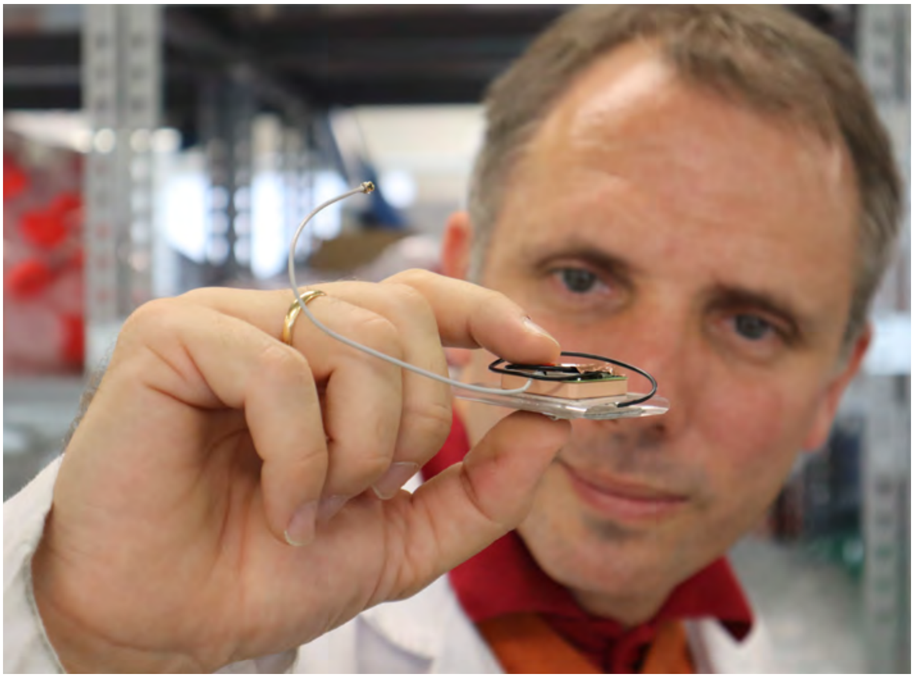
Title: VIPER (VIrtual Ply PropERty)
Description: Simulation tool developed by IMDEA Materials to predict ply properties of fiber-reinforced composite materials from the properties and spatial distribution of the different phases and interfaces in the composite.
Opportunity: Software License

Title: CAPSUL
Description: CAPSUL is a package of crystal plasticity and polycrystalline homogenisation simulation tools.
Opportunity: Commercial license through Digimat

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

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

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



“IMDEA Materials Institute Visiting Researcher, Dr. José Sánchez del Río Saéz with a prototype smark mask sensor used for monitoring a wearer’s vital signs”.

5. Training, communication and outreach

5.1. Theses

PhD Theses

1. *"Development of Flame Retardant Polymer Electrolytes for Lithium Ion Batteries"*
   Student: Abdulmalik Yusuf
   Carlos III University of Madrid
   Advisor: Dr. De-Yi Wang
   Date of defense: April, 2022

2. *"Perovskite for hybrid light emitting devices"*
   Student: Yanyan Duan
   Technical University of Madrid
   Advisor: Dr. De-Yi Wang
   Date of defense: May, 2022

3. *"Mechanical behavior of thermoplastic PEEK/PEI carbon composites"*
   Student: Sebastián Toro
   Polytechnic University of Madrid
   Advisor: Prof. Carlos González & Prof. Álvaro Ridruejo
   Date of defense: December, 2022

4. *"Computational Modeling of Powder Bed Fusion Manufacturing of Metals"*
   Student: Seyed Mohammad Elahi
   Technical University of Madrid
   Advisor: Prof. Ignacio Romero
   Date of defense: December, 2022

5. *"Constitutive Modelling and Thermomechanical Calibration of a Novel Superalloy Subjected to Extreme Conditions"*
   Student: Juan Luis de Pablos
   Technical University of Madrid
   Advisor: Prof. Ignacio Romero
   Date of defense: July, 2022

6. *"Fundamentals of solidification during selective laser melting of aerospace alloys"*
   Student: Clara Galera
   Technical University of Madrid
   Advisor: Prof. Javier LLorca
   Date of defense: May, 2022

7. *"Aerosol Jet Printing of Fibrillar Collagens for the Replication of Dense Collagenous Tissues"*
   Student: Rory Gibney
   KU Leuven
   Advisor: Dr. Eleonora Ferraris, Dr. Jennifer Patterson
   Date of defense: June, 2022

8. *"Human Stem Cell Derived Liver Cells for Disease Modeling and Whole Organ Engineering"*
   Student: Burak Toprakhisar
   KU Leuven
   Advisor: Dr. Catherine Verfaillie, Dr. Manoj Kuma, Dr. Hans Van Oosterwyck, Dr. Jennifer Patterson
   Date of defense: September, 2022

9. *"Recovery and re-use of carbon fibres from recycled end-of-life epoxy-based composites"*
   Student: Andrea Fernández
   Carlos III University of Madrid
   Advisor: Dr. Jon Molina
   Date of defense: April, 2022

10. *"Relationship between microstructure and mechanical properties in metastable beta titanium alloys and their deformation mechanisms"*
    Student: Nana Chen
    Technical University of Madrid
    Advisor: Dr. Jon Molina
    Date of defense: March, 2022

11. *"Hierarchical microstructures to overcome the conflict between strength and toughness of hard coatings: TiN/Ni as a model system"*
    Student: Ignacio López
    University of Texas in Arlington
    Advisor: Dr. Jon Molina / Prof. Efstathios Meletis
    Date of defense: June, 2022

12. *"Stable lithium-sulfur batteries through electrode and interface engineering"*
Student: Álvaro Doñoro
Autonoma University of Madrid
Advisor: Dr. V. Etacheri
Date of defense: June, 2022

13. *"Synthesis and Characterisation of Inorganic Nanowires and their Assembly into Macroscopic Structures"*
Student: Richard Schäufele
Autonoma University of Madrid
Advisor: Dr. Juan José Vilatela
Date of defense: October, 2022

Theses. Master/Bachelor Theses

1. *"Optimization of the synthesis and characterization of methacrylated gelatin for application in tissue engineering."*
Student: Álvaro Rojo
Carlos III University of Madrid
Advisor: Dr. Jennifer Patterson
Date of defense: September 2022

2. *"Resin development for 3D printing of in vitro epithelial tissue models."*
Student: Ángel Luis Camacho
Carlos III University of Madrid
Advisor: Dr. Jennifer Patterson
Date of defense: September 2022

3. *"Synthesis and physicochemical characterization of 8-armed polyethylene glycol (PEG) hydrogels for tissue engineering"*
Student: Claudia Montoro Culebradas
Carlos III University of Madrid
Advisor: Dr. Jennifer Patterson (Javier García Pérez)
Date of defense: September 2022

4. *"Development of a fracture model and characterization for a new material as structural supercapacitor"*
Student: Sergio Ramos Lozano
Rey Juan Carlos University
Advisor: Dr. Juan José Vilatela
Date of defense: July 2022

5. *"Synthesis of nanomaterials for lithium-ion battery electrodes with high energy density."*
Student: Lucía Echevarría
Complutense University of Madrid
Advisor: Dr. Maciej Haranczyk
Date of defense: June 2022

5.2. Internships / Visiting students

1. *"Functionalization of continuous carbon fiber for 3D printing application"*
Student: Helena Vermanden
Advisor: Dr. De-Yi Wang
Visiting student from: IES Palomeras de Vallecas
Period: March, 2022 – June, 2022

2. *"Design and development of hybridized and coupled nanogenerator based self-powered flexible device."*
Student: Iñaki San Félix
Advisor: Dr. De-Yi Wang
Visiting student from: International Méndez Pelayo University
Period: July, 2022 – August, 2022

3. *"Industrial Chemistry"*
Student: Lara Arranz
Advisor: Dr. De-Yi Wang
Visiting student from: IES Palomeras de Vallecas
Period: September, 2022 – January, 2023

4. *"Development of antibacterial polymer-based textiles"*
Student: Antonio Vázquez
Advisor: Dr. De-Yi Wang
Visiting student from: Rey Juan Carlos University
Period: November, 2022 – October, 2023

5. *”Chemical synthesis and nanomaterials”*
Student: Guangzhong Yin
Advisor: Dr. De-Yi Wang
Visiting student from: China University of Mining and Technology
March, 2022 – February 2023

6. *”Study of nano-carbon based materials as green flame retardant techniques to polymer-based materials”*
Student: Jie Xu
Advisor: Dr. De-Yi Wang
Visiting student from: China University of Mining and Technology
Period: October, 2022 – October, 2023

7. *“Flame retardant bio-based epoxy resin”*
Student: Meihui Zhou
Advisor: Dr. De-Yi Wang
Visiting student from: Rey Juan Carlos University
Period: March, 2022 – March 2022

8. *“Formulation of High-Performance New Biobased Fireproofing Coatings”*
Student: Pedro Luis de Hoyos
Advisor: Dr. De-Yi Wang
Visiting student from: País Vasco University
Period: January, 2022 – December, 2022

9. *“Analysis of 3D Printed Carbon Strands as Deformation Sensors”*
Student: Mario Herrerías
Advisor: Prof. Carlos González
Visiting student from: Carlos III University of Madrid
Period: September, 2022 - March, 2023

10. *“MAT 4.0”*
Student: Juan Ignacio Caballero
Advisor: Prof. Carlos González
Visiting student from: Technical University of Madrid
Period: November, 2019 - December, 2022

11. *“Combined phase field and mechanical modelling for solid-state transformations in AM Ti6Al4V alloy”*
Student: Adrián Dante Boccardo
Advisor: Dr. Damien Tourret
Visiting student from: NUI Galway
Period: June, 2021 - January, 2023

12. *“Computational investigation of oscillatory growth modes during directional solidification.”*
Student: Josep María Barberá
Advisor: Dr. Damien Tourret
Visiting student from: Technical University of Madrid
Period: June, 2022 - October, 2022

13. *“Computer simulations of phase transformations for metallurgy and nanomaterials synthesis”*
Student: Lucas Nascimiento
Advisor: Dr. Damien Tourret
Visiting student from: Federal Fluminense University
Period: June, 2022 - August, 2022

14. *“Optimal design of mechanical metamaterials with phase transitions in the elastic regime”*
Student: Nestor Oscar Rossi
Advisor: Prof. Ignacio Romero
Visiting student from: National University of Northeast
Period: November, 2022 - January, 2023

15. *“Fatigue performance of a novel lightweight steel for automotive applications”*
Student: Víctor Daniel Ortiz
Advisor: Dr. Ilchat Sabirov
Visiting student from: Complutense University of Madrid
Period: June, 2022 - September, 2022

16. *“Development and performing advanced heat treatments on a novel steel using a thermo-mechanical simulator GLEEBLE 3800”*
Student: Jiayu Li
Advisor: Dr. Ilchat Sabirov
Visiting student from: Northeastern University & Gent University
Period: December, 2022 - December, 2022

17. *"Study of microplastic deformation mechanisms of CM247LC at high temperature"*
Student: Pietro Antonio Martelli
Advisor: Dr. Ilchat Sabirov
Visiting student from: Technical University of Turin
Period: May, 2022 - August, 2022

18. *"Study of deformation and fracture mechanisms of Mg alloys in the of Mg alloys, in the framework of the HEXAGB project"*
Student: Biaobiao Yang
Advisor: Prof. Javier LLorca
Visiting student from: Technical University of Madrid
Period: December, 2021 - November, 2023

19. *"Additive manufacturing of composite materials"*
Student: Cristina Pascual
Advisor: Prof. Javier LLorca
Visiting student from: Rey Juan Carlos university
Period: October, 2020 - December, 2022

20. *"Scientific research projects"*
Student: Alejandro Elam García
Advisor: Prof. Javier LLorca
Visiting student from: DADORIS
Period: July, 2022 - July, 2022

21. *"Surface modification of biodegradable MgZnCa alloys for biomedical applications"*
Student: Emily England
Advisor: Prof. Javier LLorca and Mónica Echeverry
Visiting student from: Michigan State University
Period: June, 2022 - August, 2022

22. *"Biocompatibilty and degradation resistance of Zn alloys for biomedical applications."*
Student: Emma M. Ainsworth
Advisor: Prof. Javier LLorca
Visiting student from: Michigan State University
Period: June, 2022 - August, 2022

23. *"Develop medical grade bioabsorbable composite materials and determine the effect of degradation in vitro on the mechanical properties of the materials"*
Student: Pilar Bardisa
Advisor: Prof. Javier LLorca
Visiting student from: Technical University of Madrid
Period: October, 2022 - January, 2023

24. *"Grain boundaries in Mg alloys"*
Student: Maral Sarebanzadeh
Advisor: Prof. Javier LLorca
Visiting student from: Technical University of Madrid
Period: December, 2020 - November, 2023

25. *"Development of aminated-hydroxyetyl cellulose coatings modified with cerium oxide for magnesium alloys for biomedical applications"*
Student: Vanessa Hernández
Advisor: Prof. Javier LLorca
Visiting student from: National University of Colombia
Period: September, 2022 - February, 2023

26. *"First Principles calculations of phase diagrams"*
Student: Wei Shao
Advisor: Prof. Javier LLorca
Visiting student from: Technical University of Madrid
Period: December, 2021 - December, 2023

27. *"Sabbatical"*
Student: Jaime Marian
Advisor: Prof. Javier Segurado
Visiting student from: University of California
Period: September, 2021 - February, 2022

28. *"Synthesis and physicochemical characterization of polyethylene glycol (PEG) hydrogels for 3D bioprinting"*
Student: Claudia Montoro
Advisor: Dr. Jennifer Patterson (Javier García Pérez)
Visiting student from: Carlos III University of Madrid
Period: November, 2021 - July, 2022

29. *"Optimization of the synthesis and characterization of methacrylated gelatin for application in tissue engineering."*
Student: Álvaro Rojo
Advisor: Dr. Jennifer Patterson (Dr. Pedro Navarrete Segado)
Visiting student from: Carlos III University of Madrid
Period: December, 2021 - July, 2022

30. *"Resin development for 3D printing of in vitro epithelial tissue models."*
Student: Ángel Luis Camacho
Advisor: Dr. Jennifer Patterson (Ángela Castro María)
Visiting student from: Carlos III University of Madrid
Period: January, 2022 - August, 2022

31. *"Physicochemical characterization of hydrogel networks formed from a low molecular weight gelator"*
Student: Irene Arnaldos
Advisor: Dr. Jennifer Patterson (Javier García Pérez)
Visiting student from: InTalentia
Period: July, 2022 - September, 2022

32. *"Síntesis, caracterización y análisis de biocompatibilidad de derivados de quitosano para elaboración de hidrogeles"*
Student: Miguel Rey
Advisor: Dr. Jennifer Patterson (Shuanglan Du)
Visiting student from: Europea University of Madrid
Period: February, 2022 - July, 2022

33. *"Hard Coatings"*
Student: Álvaro Méndez Fernández
Advisor: Dr. Juan José Vilatela
Visiting student from: Nano4Energy
Period: January, 2019 - March, 2022

34. *"Surface characterization with AFM (Micromechanics Lab) of different sol-gel coatings with biomedical properties with biomedical properties"*
Student: Ángela Solís Garrido
Advisor: Dr. Miguel Monclús
Visiting student from: Carlos III University
Period: November, 2022 - December, 2022

35. *"i-MPLANTS-CM: metamaterial printing using shape memory alloys and functional gradients for a new generation of smart implants"*
Student: Carlos Aguilar Vega
Advisor: Dr. Jon Molina
Visiting student from: Technical University of Madrid
Period: November, 2022 - December, 2024

36. *"REDUTEMP"*
Student: Duwin Arley Garcia Carrero
Advisor: Dr. Jon Molina
Visiting student from: Nano4Energy
Period: December, 2022 - November, 2025

37. *"Online monitoring of SLM processes"*
Student: Giovanni Ortiz Pérez
Advisor: Dr. Jon Molina
Visiting student from: Technical University of Madrid
Period: June, 2020 - April, 2024

38. *"Enhanced plasticity of a flash sintered binderless tungsten carbide"*
Student: Isacco Mazo
Advisor: Dr. Jon Molina
Visiting student from: University of Trento
Period: June, 2021 - May, 2022

39. *"Nanoindentation of nanopatterned surfaces"*
Student: Jaime Javier Hernández Rueda
Advisor: Dr. Miguel Monclús
Visiting student from: IMDEA Nanociencia
Period: March 2018 - September, 2023

40. *"3D Printing "*
Student: José Sánchez del Río Sáez
Advisor: Dr. Jon Molina
Visiting student from: Technical University of Madrid
Period: April, 2021 - April, 2023

41. *“i-MPLANTS-CM: metamaterial printing using shape memory alloys and functional gradients for a new generation of smart implants”*
Student: Rodrigo Zapata Martínez
Advisor: Dr. Jon Molina
Visiting student from: Technical University of Madrid
Period: November, 2022 - December, 2024

42. *“Powder Metallurgy”*
Student: Alicia Páez
Advisor: Prof. José Manuel Torralba
Visiting student from: European University of Madrid
Period: April, 2022 - April, 2023

43. *“Fabricación de muestras por Composite Extrusion Modelling”*
Student: Angily Paola Cruz
Advisor: Prof. José Manuel Torralba
Visiting student from: Francisco de Paula University
Period: June, 2022 - July, 2022

44. *“Fabricación de muestras por Composite Extrusion Modelling”*
Student: Daniel Garrido
Advisor: Prof. José Manuel Torralba
Visiting student from: Carlos III University
Period: June, 2022 - July, 2022

45. *“Fabricación de muestras por Composite Extrusion Modelling”*
Student: Eduardo Tabares
Advisor: Prof. José Manuel Torralba
Visiting student from: Carlos III University
Period: June, 2022 - June, 2022

46. *“Desarrollo de aceros martensiticos formadores de alúmina”*
Student: Facundo Tomás Masari
Advisor: Prof. José Manuel Torralba
Visiting student from: Carlos III University
Period: May, 2021 - December, 2023

47. *“CoNi-based superalloy characterization”*
Student: Hailey Nicole Becker
Advisor: Prof. José Manuel Torralba
Visiting student from: University of Alabama
Period: July, 2022 - August, 2022

48. *“Heat treatment of spark plasma sintered CoNi-based high entropy superalloys”*
Student: Alessandro De Nardi
Advisor: Prof. José Manuel Torralba
Visiting student from: Carlos III University
Period: November, 2022 - June, 2023

49. *“Powder Metallurgy”*
Student: Andrea Alonso
Advisor: Prof. José Manuel Torralba
Visiting student from: Carlos III University
Period: January, 2022 - June, 2022

50. *“Flow and fracture of porous printed metals”*
Student: José Antonio Rodríguez
Advisor: Prof. José Manuel Torralba
Visiting student from: Paul Verlaine of Metz University
Period: October, 2022 - September, 2023

51. *“Síntesis de nanoestructuras 1D para conversión y almacenamiento de energía”*
Student: Isabel Gómez
Advisor: Dr. Juan José Vilatela
Visiting student from: Technical University of Madrid
Period: May, 2021 - May, 2024

52. *“Piezoresistive properties of nanostructured networks”*
Student: Ángel Víctor Labordet
Advisor: Dr. Juan José Vilatela
Visiting student from: Carlos III University of Madrid
Period: June, 2022 - August, 2022

53. *“Participation in scientific research projects”*
Student: Rafael González
Advisor: Dr. Juan José Vilatela
Visiting student from: Fundación DADORIS
Period: July, 2022 - July, 2022

54. *"Study of materials based on CNT fibers as possible soft sensors."*
Student: Lisbeth K. Mena
Advisor: Dr. Juan José Vilatela
Visiting student from: Carlos III University of Madrid
Period: December, 2022 - June, 2023

55. *"Estudio y caracterización de CNTs sintetizados mediante el método FCCVD y análisis de datos"*
Student: Raúl Fernández
Advisor: Dr. Juan José Vilatela
Visiting student from: Carlos III University of Madrid
Period: September, 2022 - July, 2023

56. *"Development of a fracture model and characterization for a new material as structural supercapacitor"*
Student: Sergio Ramos
Advisor: Dr. Juan José Vilatela
Visiting student from: InTalentia
Period: May, 2022 - December, 2022

57. *"Motion Characterisation of Nanoparticles in Elastomer-Conductive Nanoparticle Composites"*
Student: Richard J. M. Ellingham
Advisor: Dr. Juan José Vilatela
Visiting student from: University of Canterbury
Period: November, 2022 - February, 2023

58. *"Gas-phase synthesis of 1D nanowires"*
Student: Rulan Qiao
Advisor: Dr. Juan José Vilatela
Visiting student from: University of Cambridge
Period: September, 2022 - October, 2022

59. *"3D printing of lattice structures"*
Student: Sierra Green
Advisor: Teresa Pérez
Visiting student from: Massachusetts Institute of Technology
Period: June, 2022 - July, 2022

60. *"Piezoelectric behavior by finite elements modeling"*
Student: Javier Rubio
Advisor: Dr. Maciej Haranczyk
Visiting student from: Complutense University of Madrid
Period: November, 2022 - March, 2023

61. *"Development algorithms for analysis of porous structures"*
Student: Jorge Zorrilla
Advisor: Dr. Maciej Haranczyk
Visiting student from: Complutense University of Madrid
Period: January, 2021 - June, 2022

62. *"New zeolites for C2 paraffin/olefin separation"*
Student: Alechania Misturini
Advisor: Dr. Maciej Haranczyk
Visiting student from: CSIC, Institute of Chemical Technology
Period: January, 2022 - April, 2022

5.3. Teaching in Masters

1. *"Modelling and Simulation in Material Science and Engineering"*
Technical University of Madrid,
Professor: Prof. Carlos González

2. *"Design and Fabrication of Advanced Composite Materials"*
Technical University of Madrid,
Professor: Prof. Carlos González

3. *"Simulation in materials engineering"*
Technical University of Madrid,
Professor: Dr. Damien Tourret

4. *"Structural Characterization of Materials II: Spectroscopy"*
Technical University of Madrid,
Professor: Dr. Federico Sket

5. *"Advanced simulation methods*"
Technical University of Madrid,
Professor: Prof. Ignacio Romero

6. *"Advanced Strength of materials"*
Technical University of Madrid
Professor: Prof. Ignacio Romero.

7. *"Metal matrix composites*"
Technical University of Madrid/ AIRBUS
Professor: Dr. Ilchat Sabirov

8. *"Additive Manufacturing*"
Technical University of Madrid,
Professor: Dr. Jon Mikel Molina-Aldareguia

9. *"Hierarchical Composites*"
Technical University of Madrid,
Professor: Dr. Juan José Vilatela

10. *"Nanomateriales*"
Carlos III University of Madrid,
Professor: Dr. Juan José Vilatela

11. *"Thermal and Thermo-mechanical characterization*"
Carlos III University of Madrid,
Professor: Dr. Srdjan Milenkovic

12. *"Additive Manufacturing"*
Navarra University
Dr. María Teresa Pérez-Prado

5.4. Institutional activities

1. *Member of the Advanced Materials 2030 Initiative (AMI2030). Prof. José Manuel Torralba*
2. *Member of the European Technology Platform for Advanced Engineering Materials and Technologies (EUMAT)*
3. *Member of the Batteries European Partnership Association (BEPA). Dr. Juan José Vilatela*
4. *Member of the European Energy Research Alliance (EERA). Prof. Javier LLorca*
5. *Member of the European Aeronautics Science Network (EASN). Prof. Javier LLorca*
6. *Member of the European Technology and Innovation Platform Batteries Europe. Dr. Juan José Vilatela*
7. *Member of the European Powder Metallurgy Association (EPMA). Dr. María Teresa Pérez-Prado*
8. *Member of the Spanish Association of Composite Materials (AEMAC). Prof. Carlos González*
9. *Member of the Severo Ochoa and María de Maetzu Units Alliance (SOMMA)*
10. *Technical Secretariat of the Spanish Technological Platform of Advanced Materials and Nanomaterials (MATERPLAT)*
11. *Member of the Spanish Aerospace Technology Platform (PAE)*
12. *Member of the Spanish Technological Platform for Advanced Manufacturing (MANUKET)*
13. *Member of the Spanish Railway Technological Platform (PTFE)*
14. *Member of the Spanish Energy Storage Technological Platform (BATTERYPLAT)*
15. *Member of the Spanish Materials Society (SOCIEMAT)*
16. *Member of the Madrid Aerospace Cluster (MAC)*
17. *Local Contact Point of the EURAXESS Network*

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

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

5.5. Outreach

1. *Participation in the debate "The use of for sustainable mobility", M.T. Pérez-Prado. February, 2022.*

2. *Organisation of the "3rd open PhD day". IMDEA Materials Institute. March, 2022.*

3. *Organisation of the "1st edition of THESIS TALK: 3MT". IMDEA Materials Institute. March, 2022.*

4. *Participation in the Fair "Madrid is Science", M. Echeverry, C. Martínez Alonso, J. García-Pérez, J. Hobson, X. Lin, I. Escobar, I. Rodríguez-Barber, G. Domínguez, X. Ao, J. de la Vega, C. Thompson, A. K. Boukellal, S. Liu, Á. Castro, A. Gomez, M.T. Pérez-Prado. Madrid. March, 2022*

5. *Participation in "Falling Walls Lab Spain 2022" – Novel Additive Manufacturing, Venkatesh Kumaran. Madrid. June, 2022.*

6. *Participation in "European Researchers' night - The five EU Missions seen by IMDEA researchers" (I), L. Martín, I. Gomez. Madrid. September, 2022.*

7. *Participation in the "Science Week of Madrid", D. Mocerino, J. Fernández, I. Gómez, L. Arevalo, A. Castro, C. Thomson. November 2022.*

8. *Organisation of primary-secondary school and bachelor-master students visits to IMDEA Materials, 10 visits during 2022 with over 160 visitors.*

IMDEA Materials Institute Media Appearances:

• *IMDEA Materials Institute appearances on television: 3*

• *IMDEA Materials Institute appearances on radio: 6*

• *IMDEA Materials Institute appearances in general print media: 13*

• *IMDEA Materials Institute appearances in trade publications: 11*

IMDEA Materials researchers participating in the annual Madrid is Science Fair as part of the Institute's outreach activities.

IMDEA Materials In the Media

All the news from 2022

actualidad aeroespacial
EL PORTAL DE LOS PROFESIONALES DE LA AERONÁUTICA Y EL ESPACIO

IMDEA Materials technology will revolutionise airspace manufacture

27/4/2022

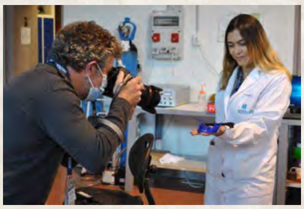
Advances in carbon nanotube (CNT) fiber technology at the Madrid Institute for Advanced Materials Studies (IMDEA Materials) could prove crucial in the aerospace industry.

https://actualidadaeroespacial.com/la-tecnologia-de-imdea-materiales-revolucionara-la-fabricacion-aeroespacial/?utm_source=mailpoet&utm_medium=email&utm_campaign=actualidad-aeroespacial-28%2F04%2F2022

EL MUNDO

The medicine of the future is 'cooking' in Madrid: from customised prostheses to those that disappear after healing

13/6/2022



A leading research center of the Community of Madrid is working on discovering new materials that are already paving the way for the production of customized and biodegradable prostheses.

In the area of Tissue Engineering and Regenerative Medicine, bioengineer Mónica Echeverry is working - under the orders of Javier Llorca - on several lines of research that in the near future will lead hospitals to offer 100% personalized medicine.

https://www.elmundo.es/madrid/2022/06/13/629757ade4d4d8ca038b45b8.html

ABC

The Engineer who hung up her boots for the love of science

23/06/2022

Between playing in the first division or being a researcher, Lola Martín opted for the latter. On the International Day of Women in Engineering, her case reflects the unstoppable change in this sector.

https://www.abc.es/espana/madrid/abci-ingeniera-colgo-botas-amor-ciencia-202206230137_noticia.html

Prof José Torralba to receive 2022 Ivor Jenkins Medal

POWDER METALLURGY REVIEW

14/6/2022

IOM3 has announced that Prof Jose Manuel Torralba, Director, IMDEA Materials Institute, has been awarded the 2022 Ivor Jenkins Medal. The prestigious award is presented to individuals in recognition of a significant contribution that has enhanced the scientific, industrial or technological understanding of materials processing or component production using Powder Metallurgy and particulate materials.

https://www.pm-review.com/prof-jose-torralba-to-receive-2022-ivor-jenkins-medal/

IMDEA Materials of Getafe researches the creation of biodegradable prostheses for the human body

SER

18/8/2022

IMDEA Materials, one of the seven Madrid Institutes of Advanced Studies, has started this past July an ambitious European research to develop biodegradable materials inside the human body to create prostheses and implants that disappear over time, without the need for further surgery.

https://cadenaser.com/cmadrid/2022/08/18/el-imdea-materiales-de-getafe-investiga-la-creacion-de-protesis-biodegradables-para-el-cuerpo-humano-ser-madrid-sur/

The chemistry of poetry

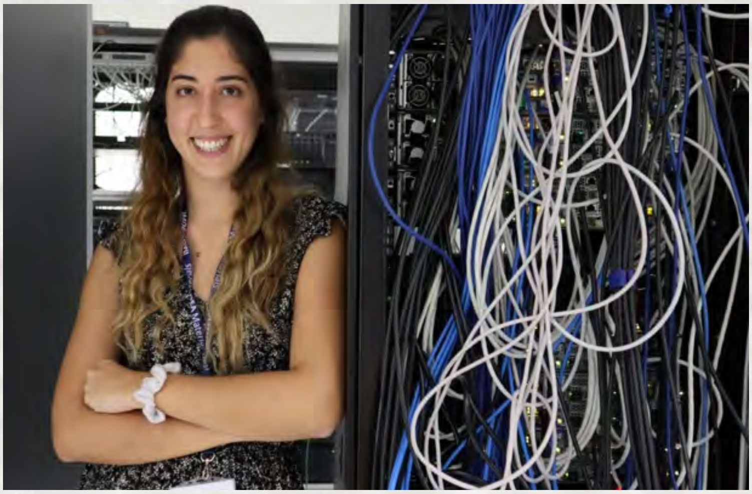
EL MUNDO

28/7/2022

Her profile is unconventional. She loves science and literature in equal parts. Carmen Martínez Alonso, from Burgos, studied chemistry because she finds it an exciting discipline of knowledge; however, she recognizes that she has been falling in love with it little by little. In fact, when she had to choose a career she hesitated, and even considered studying philosophy.

She discarded it, although he is currently studying a degree in Spanish Language and Literature at the Universidad Nacional de Educación a Distancia (UNED). In this sense, she says that literature is a part of her. She has been writing poetry and attending literary gatherings since she was 14 years old..

https://diariodecastillayleon.elmundo.es/articulo/innovadores/quimica-poesias/20220714115410051955.html



IMDEA Materials Institute helps create intelligent sensors for aviation composites

CW CompositesWorld

12/9/2022

IMDEA Materials Institute (Madrid, Spain) is playing a key role in the development of next-generation aircraft sensor technology which will enable real-time monitoring of airframe components in flight.

Such smart sensors, designed to be embedded within the parts themselves, are set to provide benefits in both cost and safety to the airline industry in the coming years (learn more about sensors in composites).

This, at least, is one of the goals of the European Union-funded Digital Method for Improved Manufacturing of Next-Generation Multifunctional Airframe Parts (DOMMINIO) project.

https://www.compositesworld.com/news/imdea-materials-institute-helps-create-intelligent-sensors-for-aviation-composites

An IMDEA Materials project could save babies' lives

TeleMadrid

06/08/2022

A new project at the Institute of Advanced Studies in Madrid has developed a new technique to treat craniostenosis, a disease that closes the bones of the skull prematurely, affecting one in every two thousand newborns.

https://www.telemadrid.es/programas/telenoticias-fin-de-semana/Un-proyecto-del-Instituto-de-Estudios-Avanzados-de-Madrid-podria-salvar-la-vida-de-bebes-2-2475672414--20220806040601.html

Whoever controls the materials of the future will rule the world

20minutos

28/9/2022

Elinvar is a unicorn, a new material that seemed impossible, created by humans using principles bordering on magic that allow high entropy alloys to exist. Elinvar has an exceptional property that throws any textbook to the wind: it is a metal that increases in rigidity when heated. Where are we going to use it?

https://www.20minutos.es/tecnologia/actualidad/quien-controle-los-materiales-venideros-dominara-el-mundo-que-son-las-aleaciones-de-alta-entropia-5064118/

New smart mask designed to revolutionize the market

ConSalud.es

9/11/2022

A group of researchers have developed and patented a novel intelligent mask that, thanks to its innovative design, allows a series of vital parameters to be monitored from up to 20 kilometers away. This mask is the result of the "Materials and Models Against Pandemics (MAMAP-CM)" project, funded by the Community of Madrid and a collaboration between IMDEA Materials, the Polytechnic University of Madrid (UPM) and the Rey Juan Carlos University (URJC).

https://www.consalud.es/tecnologia/tecnologia-sanitaria/nuevos-modelos-mascarillas-inteligentes_122570_102.html

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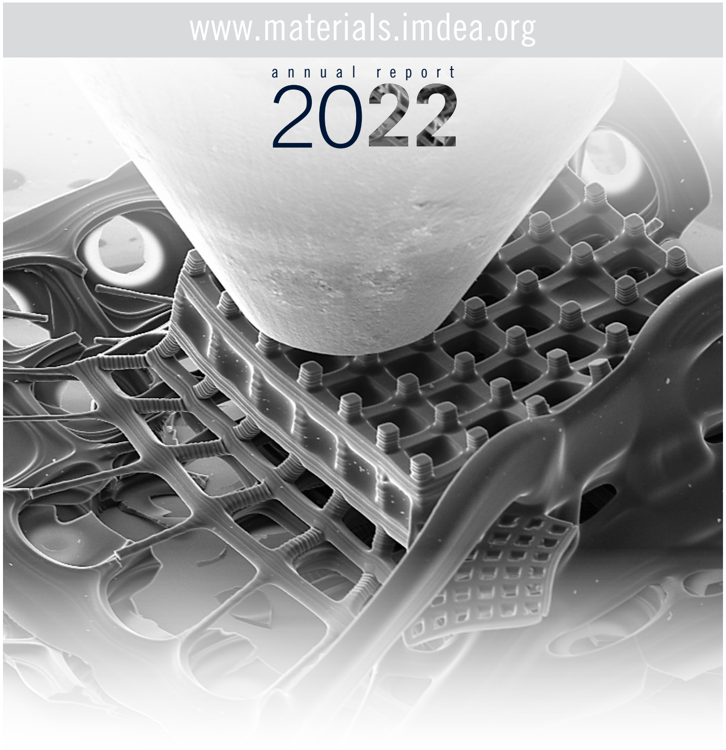
STRUCTURAL FUNDS



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