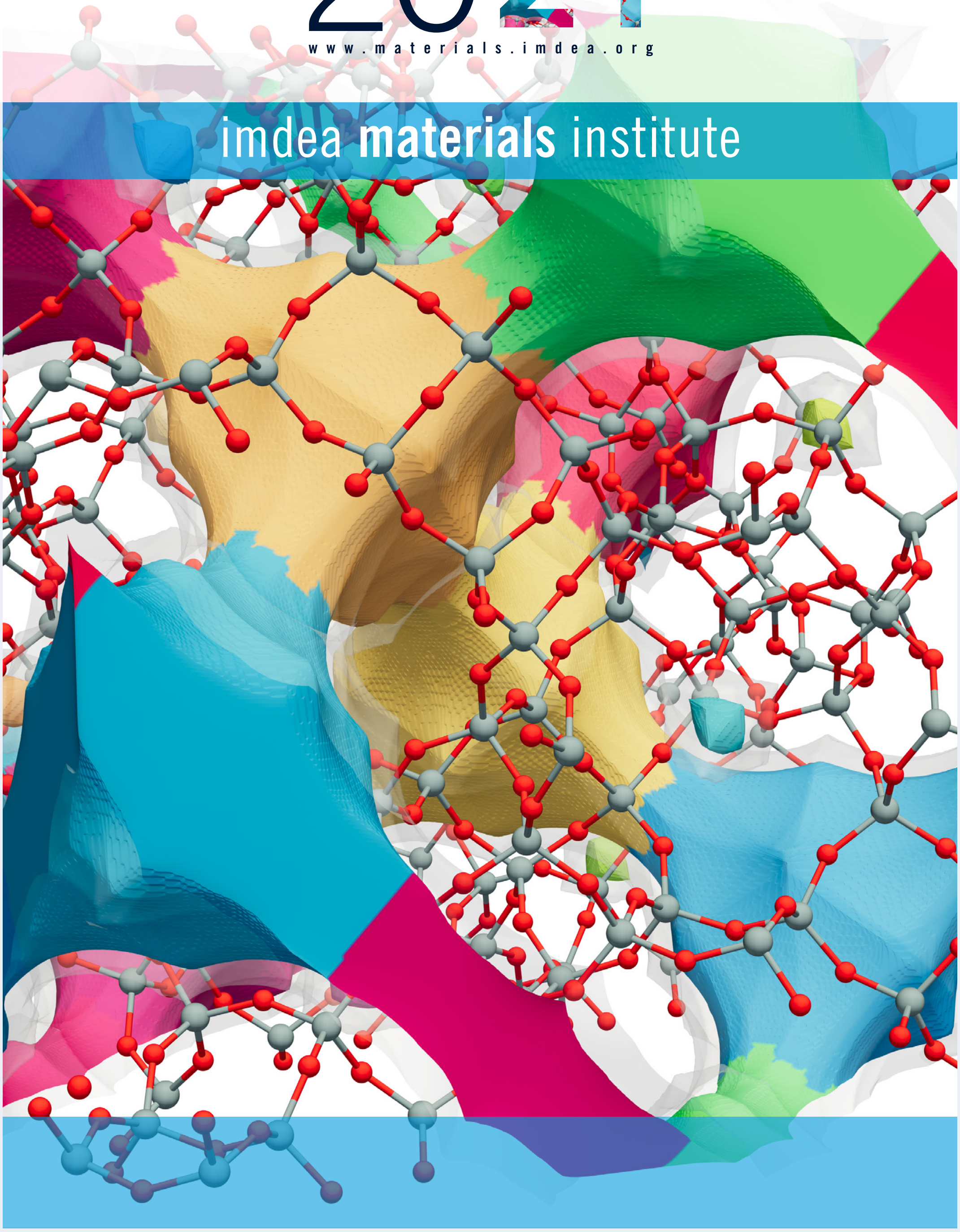
annual report 2021

www.materials.imdea.org



institute imdea materials

José Manuel Torralba
Director, IMDEA Materials Institute
June 2022

annual report
2021
www.materials.imdea.org

When writing these lines, the sixth wave of COVID19 is long gone, and we are approaching a situation of normality. When it seemed that our lives were returning to that normality, the invasion of Ukraine by Russia, and the associated humanitarian catastrophe, together with the strengthening of the economic crisis in which the pandemic left us, made us return to a situation of enormous uncertainty. But it is time to reflect on how IMDEA Materials performed in 2021, the year I have had the honour of assuming the Directorate of the Institute after a long selection process. I took over from Prof. Ignacio Romero, who carried out this work so well during the challenging last few years. My first lines have to be of gratitude to him and his Deputy Director, Dr. Teresa Pérez-Prado, for the dedication and the vital boost they have given the Institute in fulfilling its mission.

Speaking of that mission, the year 2021 can be considered very positive in performance. It has been a year in which science of excellence has continued to be carried out (the first pillar of our Institute), already under the “María de Maeztu” distinction, which recognizes us as a center of excellence by our State Research Agency (AEI). 12 new research projects started along the year (8 of which are competitive grants, including 2 from the European Union Framework Programme), and 9 new researchers joined the Institute through competitive fellowships, all representing an amount of 4 million euros executed in 2021. This new income from projects and fellowships means that IMDEA Materials currently manages 61 active R&D projects and 37 fellowships. This success in attracting external funds means that the percentage of our budget for the regional government’s baseline funding is close to 40%, which is a significant effort in the Spanish environment. Our researchers have continued to produce quality papers (125 in top-level journals), currently supervise 61 PhD theses, delivered 36 plenary or keynote presentations at international conferences and 9 invited lectures at prestigious international centers. Our new “Materials for Health Care” research line is gaining strength and has contributed significantly to these figures. All this reflects our commitment to the first pillar of our mission, developing science of excellence.

Relevant events have also occurred in 2021 linked to the third pillar of our mission (technology transfer to industry) that should make us all proud. We have strengthened ties and collaboration with some of our strategic industrial partners. We also launched our Industrial Advisory Board, which we think will help reinforce this pillar. Finally, and above all, we launched our first spin-off, Floathech, promoted by our researchers Juan José Vilatela and Richard Schäufele. These are also important milestones in our growth.

And if we have tried to improve our performance in the last two pillars of our mission, we have also strengthened the last one: talent attraction. Currently, the Institute has its highest historical ratio of Doctorates from foreign universities (75%). We continue to believe that talent is our primary value and that attracting the best talent allows us to succeed in achieving science of excellence and technology transfer. We also launched our gender equality plan and remain committed to following our code of ethics and promoting a culture of compliance.

2021 has been another challenging year, tempered by the pandemic. But we have worked hard to maintain the demanding performance levels expected of IMDEA Materials. As we walk through the Institute’s main door every morning, a plaque reminds us that we are a “María de Maeztu” center of excellence. And that is undoubtedly an incentive for us to be non-conformists with our current performance and seek much more. We have a bright future ahead of us.

words from the director...

annual report

2021

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editor

IMDEA Materials Institute

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cover picture

Jorge Zorrilla. Winner of the imaging contest 2022 (simulation)

contents

about us

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

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

mission

We do research of excellence in Materials Science, contributing to tackle the challenges of society and fostering the sustainable development of the region of Madrid.

vision

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

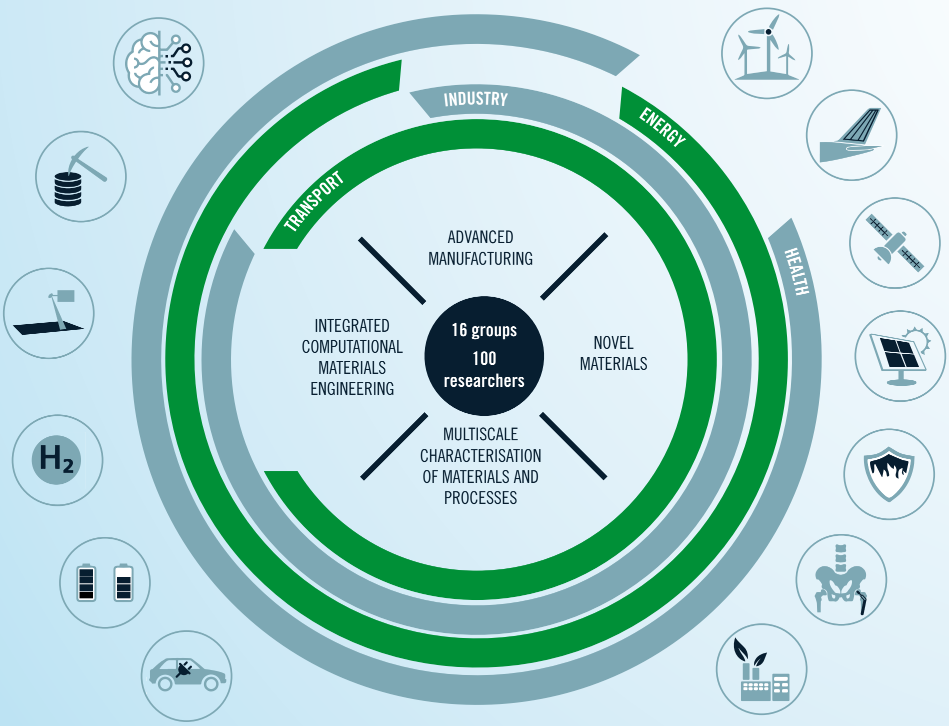
The mission and vision of the IMDEA Materials Institute is based in three main pillars:

science — **excellence** in materials **science** and engineering research

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

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

SECTORS AND AREAS OF APPLICATION



RESEARCH PROGRAMMES

Novel Materials

Advanced Manufacturing

Integrated Computational Materials Engineering

Multiscale Characterisation of Materials and Processes

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

100 researchers, 23 nationalities, 37% PhDs, 56% foreign researchers
16 research groups

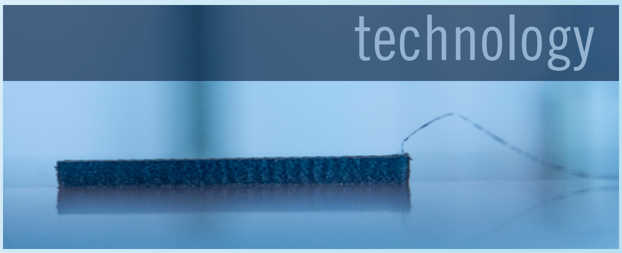
The facilities of IMDEA Materials Institute
The building and laboratories of IMDEA Materials Institute are located at the Scientific and Technological Park of the Technical University of Madrid in Tecnogetafe, Madrid.

2.640 m^2 of research labs

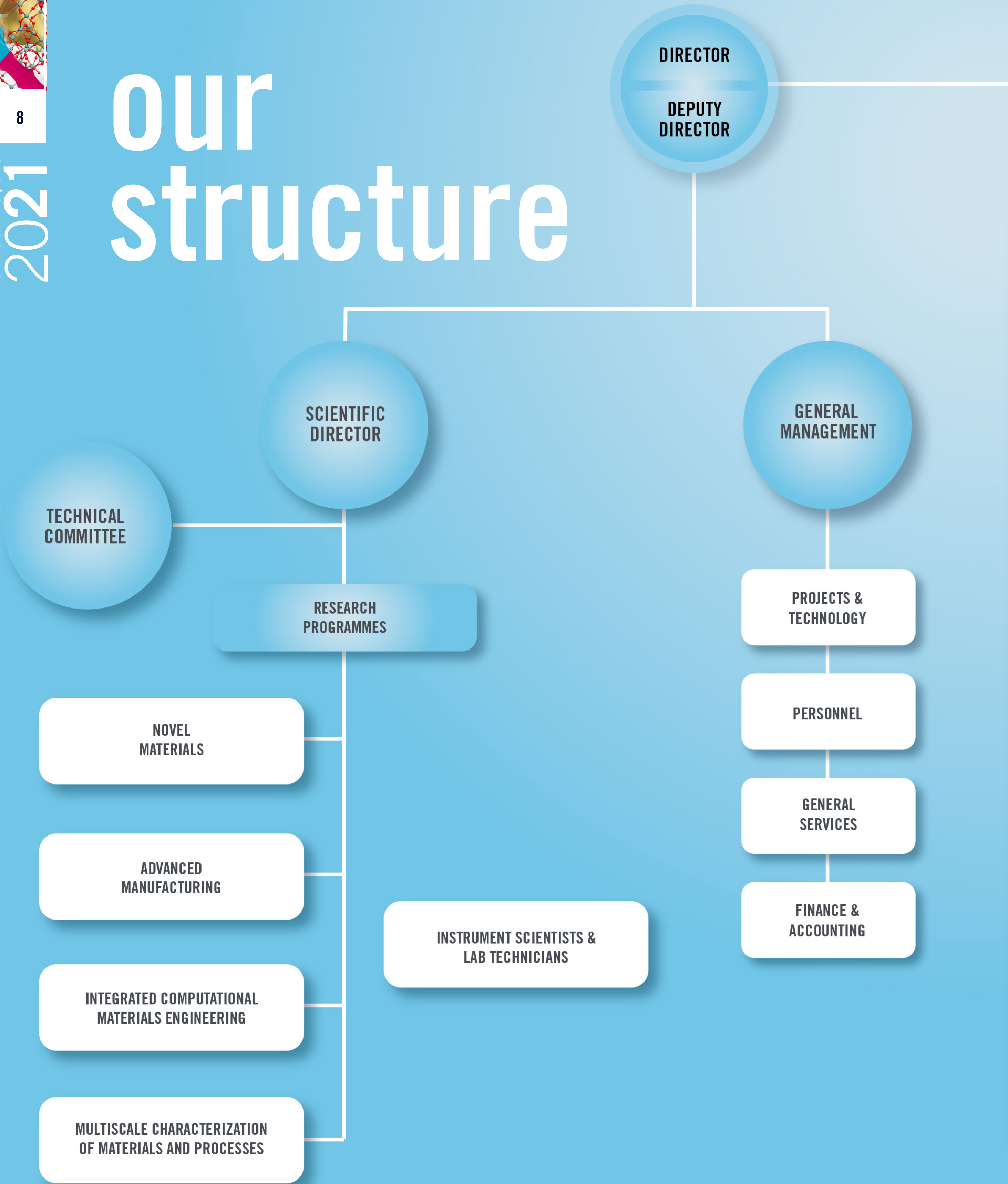
Auditorium (200 people) and networking space for international Conferences and Workshops.

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

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



our structure



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Hexagon HMI

in figures

human resources

talent

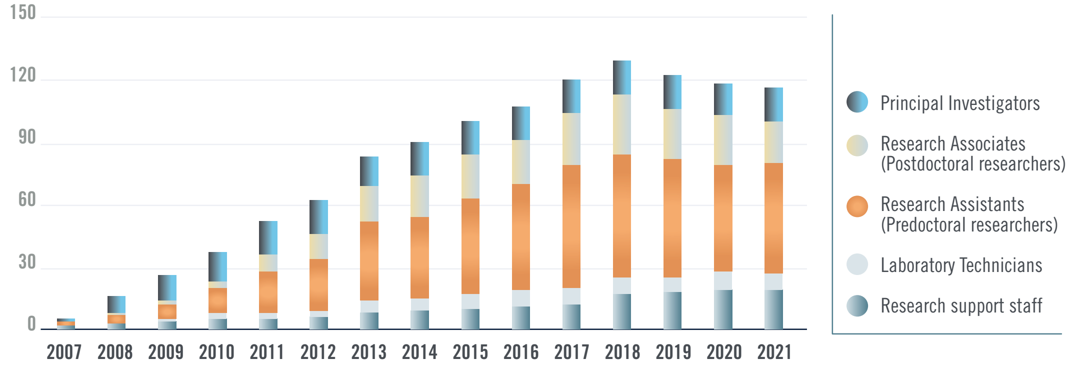
Talent attraction has been the key to the Institute´s **success**.

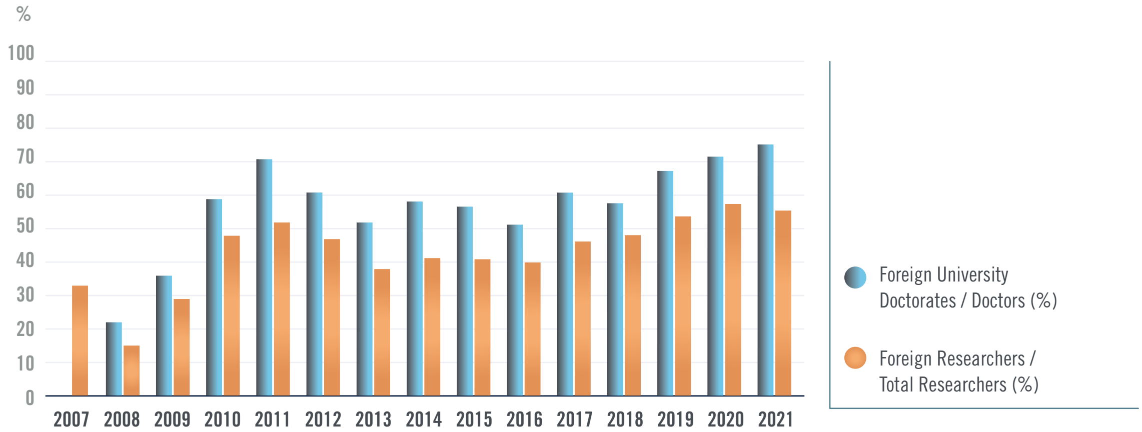
Open and transparent selection along with regular evaluation of principal investigators performed by an independent **Scientific Council.**

hr
HR EXCELLENCE IN RESEARCH

IMDEA Materials has created a **multidisciplinary and international working environment** to attract and maintain talented researchers from all over the world.

Career development at IMDEA Materials is acknowledged by the EU´s HR excellence in research seal.





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

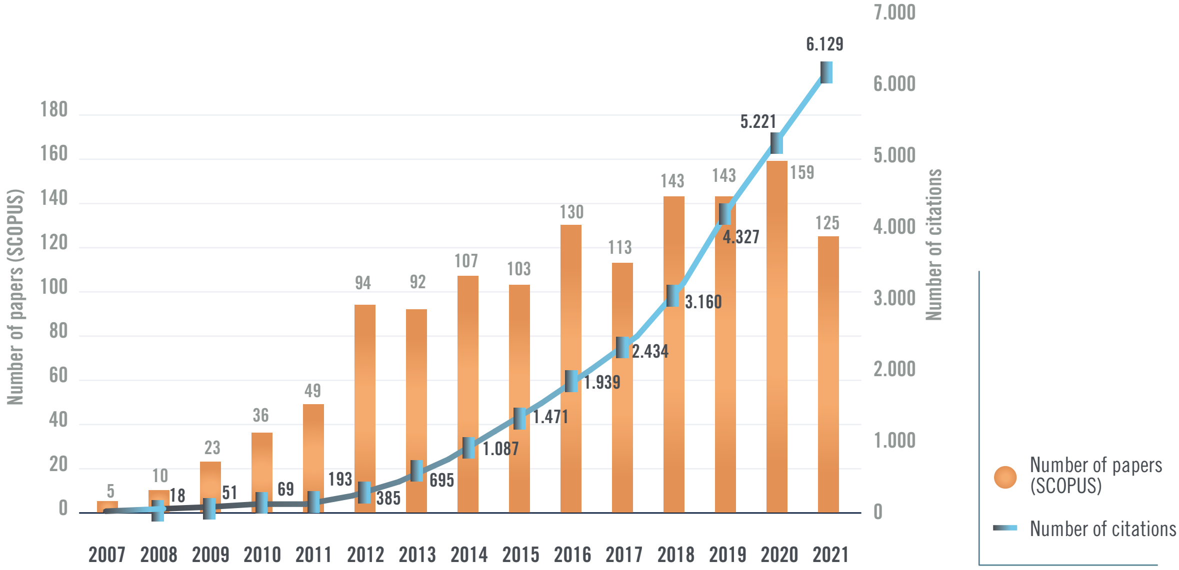
76 defended PhD theses since 2007

61 ongoing PhD theses

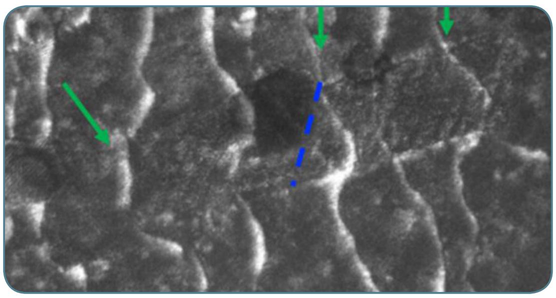
scientific results

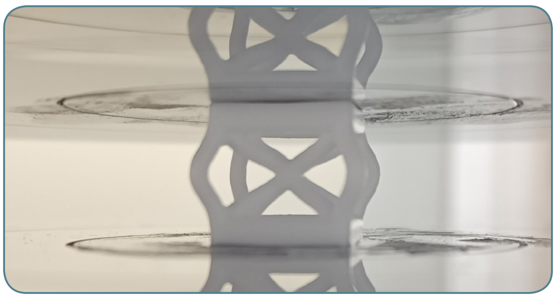
science

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



2021





36
keynote/
invited talks

125
papers
(SCOPUS)

6129
citations

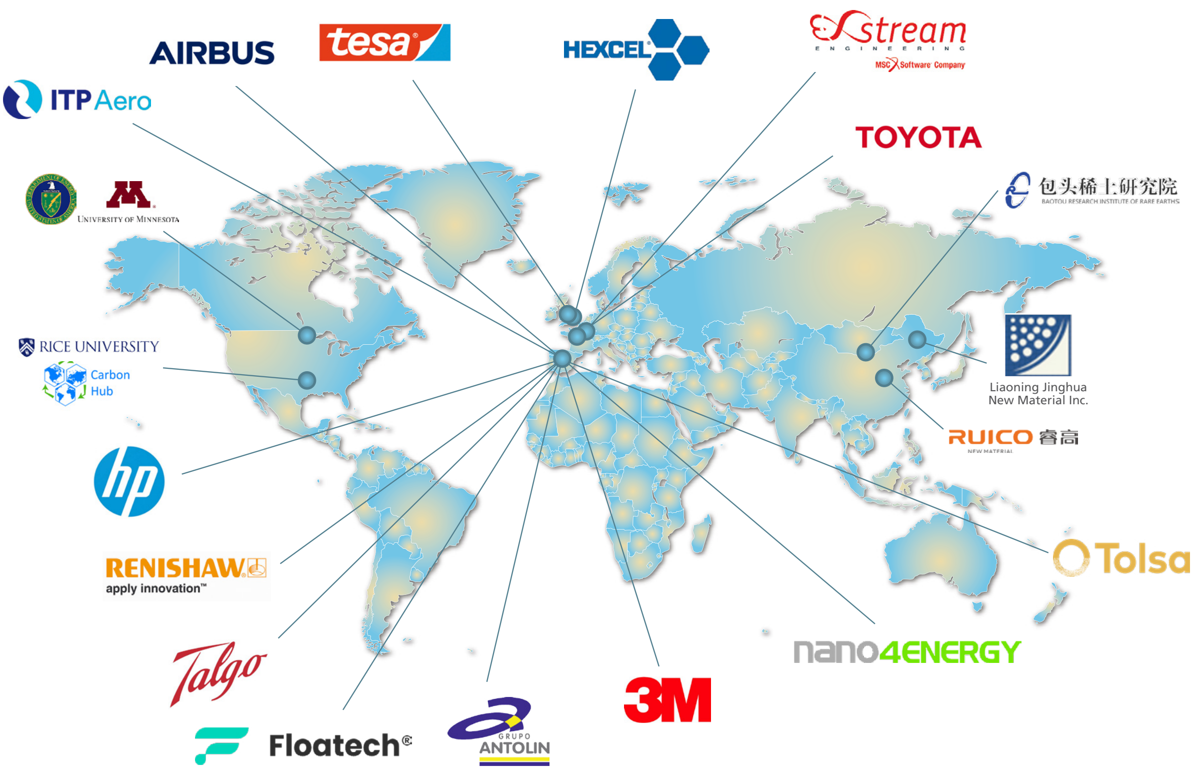
9
invited
seminars
and lectures

technology transfer and innovation

transfer

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

Companies which had active collaborations with the IMDEA Materials Institute in 2021:

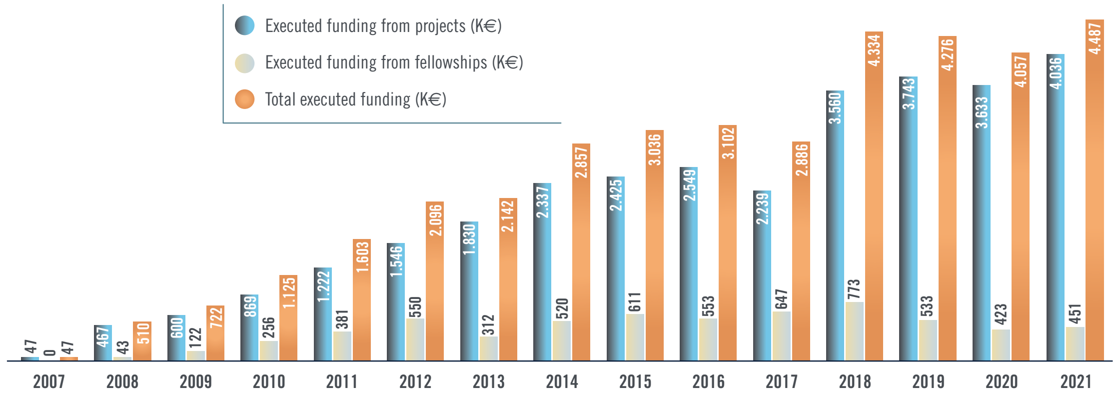


Performance indicators in 2021

- **18** Bilateral projects with industry
- **4** Industrial doctorates
- **2** Patent applications
- **11** Patents in portfolio (granted and under evaluation)
- **2** Patents licensed
- **5** Software tools registered in portfolio
- **2** Software tools licensed
- **1** **Valorisation project:** (SiNERGY) Silicon nanowire fabrics for high energy density batteries
- **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.



2021

International projects
36%

National projects
35%

Regional projects
16%

Contracts with industry
13%

61
R&D projects

3
Active ERC projects

1
Active FET open projects

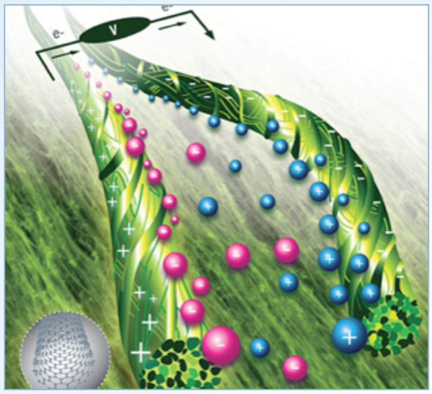
research

talent **science** **transfer**

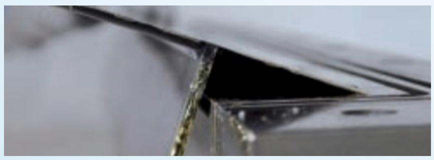
The Institute is currently organised into sixteen **research groups** focused on different areas in the field of Materials Science and Engineering. Each of these groups is led by one staff researcher, who is in charge of coordinating and supervising a research team of post and predoctoral reseachers.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

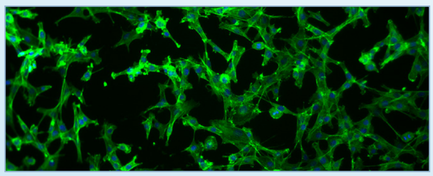
As a result of a high degree of internal collaboration, each research group at the IMDEA Materials Institute participates in several of our **research programmes**. Driven by the talent of the researchers, the research programmes combine cutting-edge fundamental oriented research in topics at the frontiers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

Novel Materials



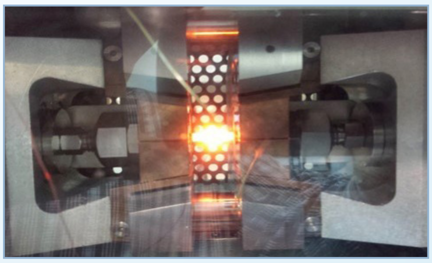
- Synthesis and integration of nanomaterials
- Synthesis and properties of polymer-based multifunctional nanocomposites
- Materials for hydrogen economy
- Metallic materials
- Materials for extreme conditions
- Materials for Lithium-Ion Batteries (LIBs)
- Materials for post LIBs
- Lightweight materials
- Green materials approaches
- Regenerative engineering
- Medical treatments

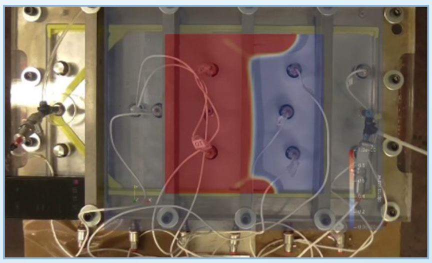




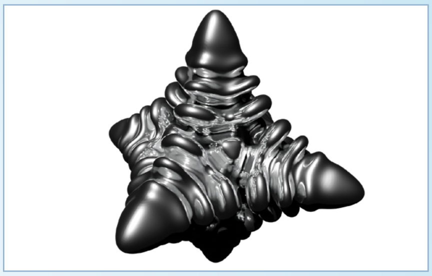
Advanced Manufacturing

- Industry 4.0
- Bulk nanostructured materials
- Liquid and solid-state processing
- 3D printing

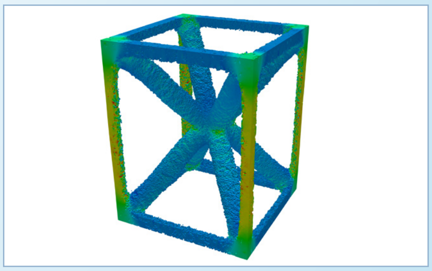


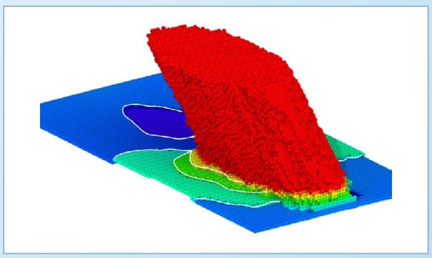


Integrated Computational Materials Engineering

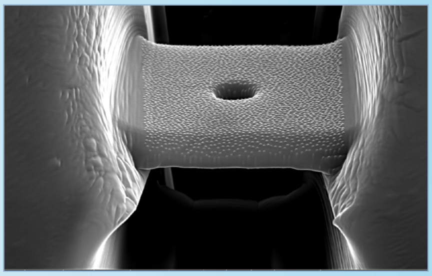


- Virtual materials design, including virtual processing and virtual testing
- Materials modelling at different length and time scales
- Multiscale materials modelling
- Modelling and simulation strategies for different applications
- Computational and data-driven materials discovery

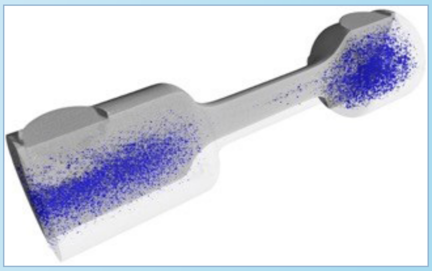


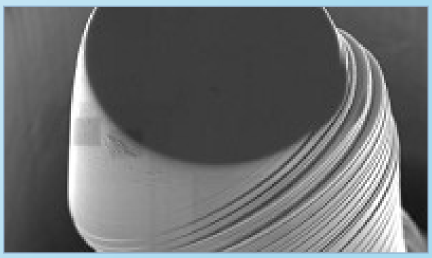


Multiscale Characterisation of Materials and Processes



- 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,...)



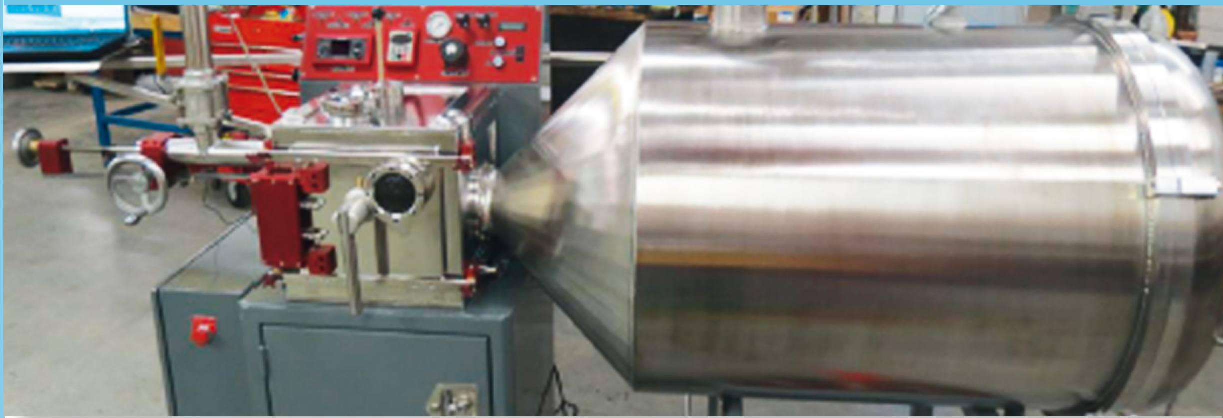


facilities

talent science transfer

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

Synthesis, processing and integration of materials



Metallic alloys

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

Polymer based composites and nanocomposites

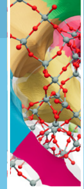
- Liquid moulding processing: RTM resin transfer moulding, VI vacuum infusion, RFI resin film infusion and pultrusion.
- Prepreg lamination using vacuum bagging of autoclave and out-of-autoclave prepregs (OoA) or laminate hot-press moulding (<400°C).
- Semi-industrial equipment for compounding and injection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

Nanomaterials

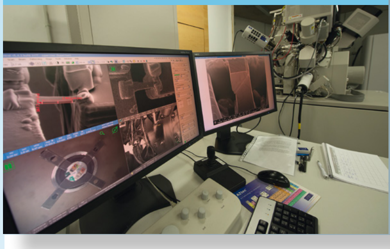
- Synthesis and chemical modification of nanocarbons, inorganic materials, nanoporous semiconductors, thin films, zeolites and other nanomaterials.
- Evaporation equipment in controlled atmospheres, high-pressure reactors and in-house chemical vapour deposition systems.

Energy storage and conversion devices

- Synthesis and characterisation of nanostructured electrode materials for energy storage applications. Fabrication of composite electrodes and integration in various types of rechargeable batteries (Li-ion, Li-S, Li-O_2, Na-ion, and hybrid batteries etc.).
- Fabrication and testing of nanocarbon-based electrodes and their integration with liquid and solid electrolytes to form large-age (> 100 cm^2) flexible supercapacitors.
- Integration of energy-storage functions in structural composites
- Fabrication (solvent-based deposition, physical vapour deposition, high temperature sintering ovens and hot plates) and characterization (solar simulators, incident photon-to-current conversion, electrochemical impedance spectroscopy and intensity-modulated photovoltage spectroscopy) of hybrid solar cells and thin-film organic solar cells.

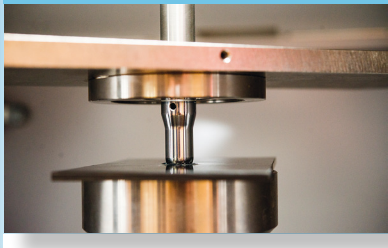


Microstructural and chemical characterisation



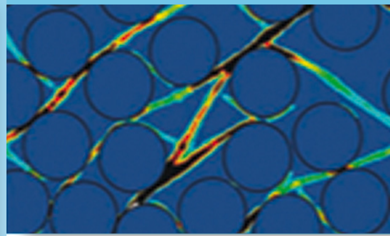
- 3D microscopy at different length-scales, including X-ray tomography, X-ray diffraction, 3D-SEM, 3D-EDS and 3D-EBSD in the FIB, and 3D-TEM and 3D-EDS in the TEM.
- In-situ thermos-mechanical testing of mininaturised samples in the X-ray tomography system, as well as in the SEM and TEM.
- In-situ processing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

Mechanical properties



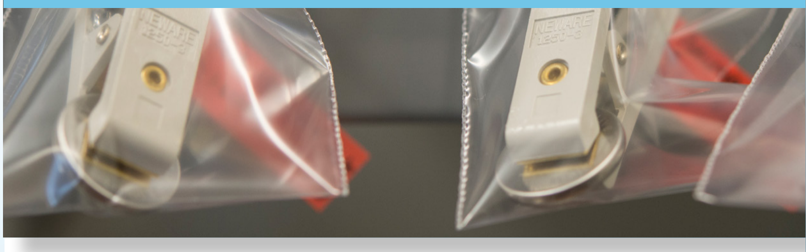
- Mechanical testing of a wide range of materials, using electromechanical and hydraulic machines (quasi-static, dynamic, fracture and fatigue testing in a wide range of temperatures).
- Characterisation of mechanical properties at multiple length scales, including nanoindentation, micropillar compression,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

Simulation



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

Functional properties



Fire resistance

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

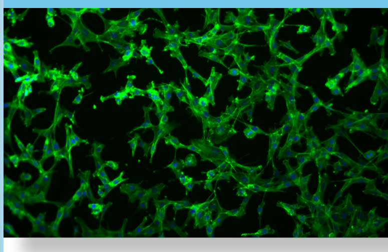
Thermal

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

Electrochemical

- Electrochemical characterisation of energy storage devices (Li-ion, Li-S, Li-O_2, Na-ion, and hybrid batteries). Simultaneous testing of 100 batteries can be performed using multichannel battery testers.
- Galvanostatic/potentiostatic cycling at various current densities.
- Single channel Zive SP1 electrochemical workstation is used for cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) study of batteries.
- LCR equipment to quantify dielectric properties in composites.

Biomaterials and cell culture

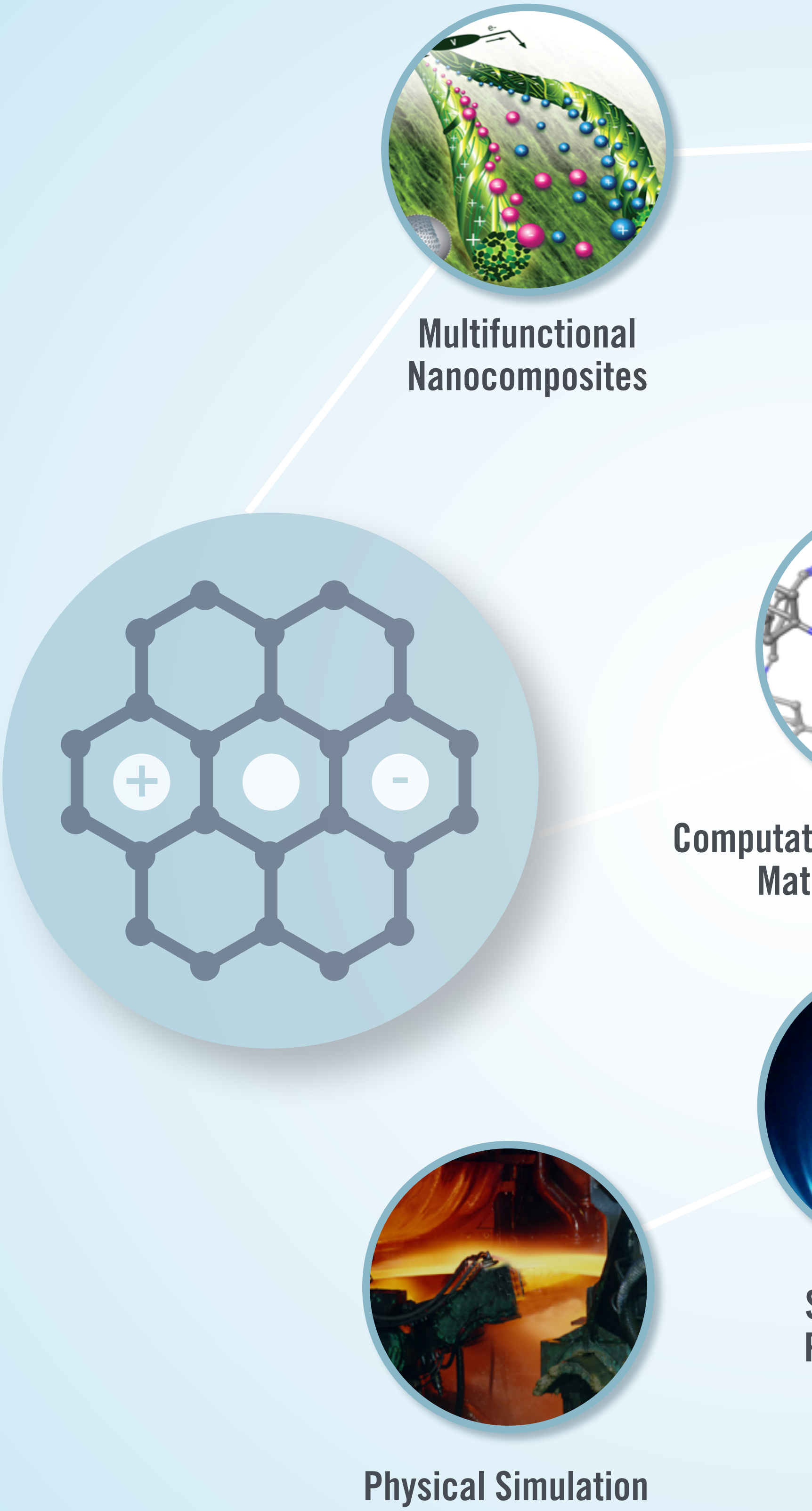


- Confocal, fluorescence and inverted microscopes
- PCR instrument
- Multi-mode plate reader (absorbance, fluorescence, luminescence)
- Ultrasonic processor
- Autoclave
- Protein gel electrophoresis and blotting system
- Liquid nitrogen tank for cell storage and -80 ºC freezer
- Prusa mini 3D printer
- Biosafety cabinets
- Benchtop and CO_2 incubators
- Centrifuge and microcentrifugue, vortex mixers, hot plate stirrer, dry block heater, UV lamp, and thermostatic water baths

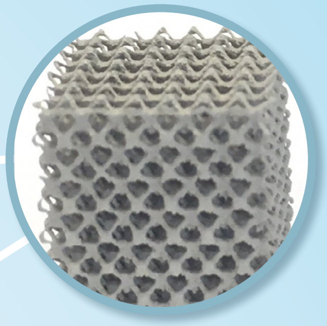
programme
Novel Materials

Goal and vision

The programme on Novel Materials combines expertise in design and synthesis of nano and molecular building blocks with their integration into macroscopic materials and devices, in developing solutions for high-performance structural composites with enhanced multifunctional capabilities such as thermal, electrical and fire resistance, and in exploring the processing-structure-property relationship 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.

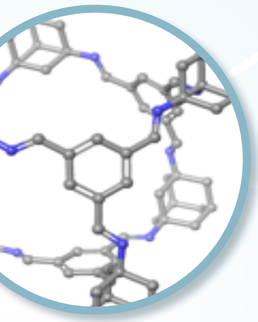


High Performance Polymer Nanocomposites



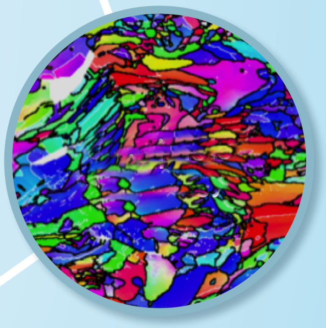
Bio/Chemo/Mechanics of Materials

Structural composites

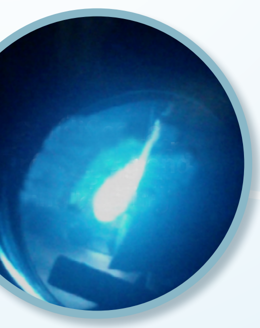


ional and Data-Driven erials Discovery

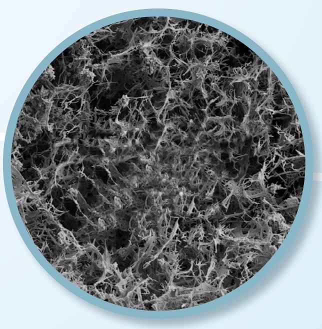
Nanomechanics and Micromechanics



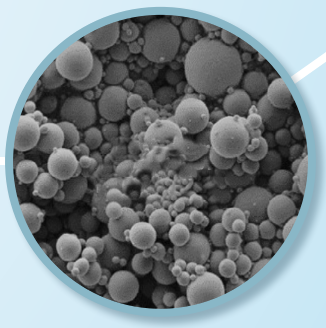
Sustainable Metallurgy



Solidification Processing & Engineering



Biomaterials and Regenerative Medicine



Sustainable Powder Metallurgy

Main research lines

Synthesis and integration of nanomaterials (nanotubes, nanofibers, MXene, quantum dots, graphene, and hybrids)

- 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.

Metallic materials

- Advanced high strength steels showing 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.

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.

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

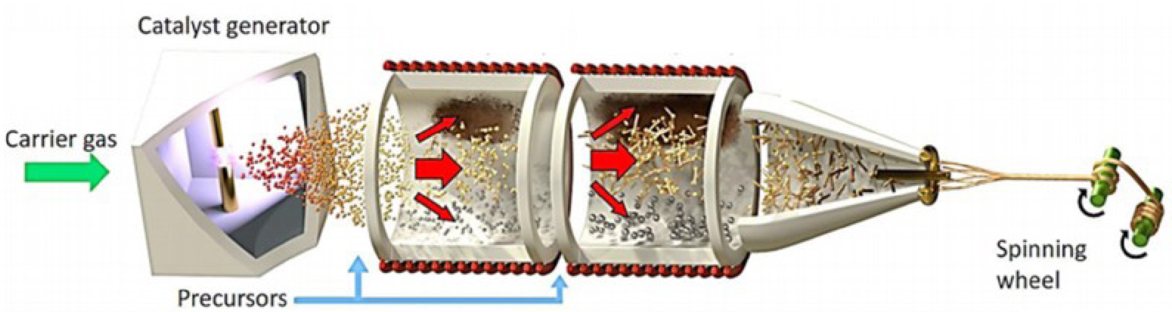
- Bio-based polymers fibres and additives.
- Reprocessable composites.
- Valorization of by-products in hydrogen production.
- Biobased thermal energy storage/phase change materials

Regenerative engineering

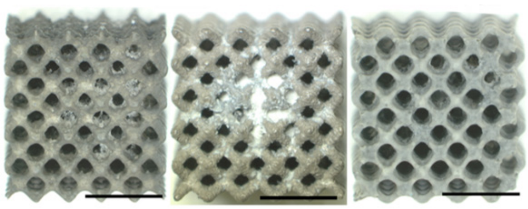
- Bioresorbable 3D printed metallic and composite scaffolds for bone regeneration.
- New materials for tissue engineering and regenerative medicine.
- Biodegradable cardiovascular metallic stents via 3D printing.

Medical treatments

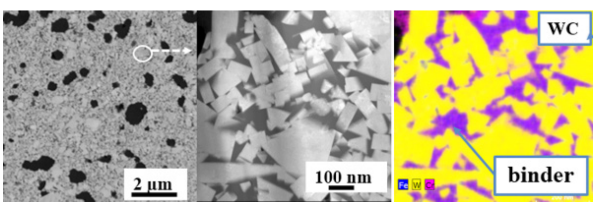
- Degradable metal nanoparticles for biomedical applications (anticancer or antibacterial activity).
- Biofunctionalization and surface modification on materials with molecules to improve their performance.
- Mechanotransduction.



Schematic of the synthesis of 1D nanomaterials via a floating catalyst.



3D printed Mg scaffolds for bioresorbable bone implants



New cemented carbides Cr-Fe based nano-reinforced

Projects in focus

i-MPLANTS-CM / Metamaterial printing using shape memory alloys and functional gradients for a new generation of smart implants

Funding: Regional Government of Madrid/Synergy projects
Partners: Technical University of Madrid (Coordinator) and IMDEA Materials Institute
Project period: 2021 - 2024
Principal Investigator: Dr. J. M. Molina-Aldareguia

This project pursues the development of a new generation of intelligent implants, which will be implanted through minimally invasive procedures and will be able to evolve geometrically with the patients, shifting their shapes, according to the healing, growth and ageing processes (see Figure 1). To this end, it is necessary to investigate and develop principles and techniques for the design and additive manufacturing of metamaterials, using shape memory alloys as raw materials and employing functional gradients, whose innovative structures, biomechanical properties and metamorphic abilities will enable novel interactions with patients.

The advances of the i-MPLANTS-CM project will be illustrated with case studies from the cardiovascular realm, by means of designs, prototyping and validation trials of real implants including unconventional stents for the personalized treatment of complex aneurysms in arterial bifurcations and minimally invasive artificial heart valves with shape morphing capabilities.

Combined employment of metamaterials, with singular properties derived from their microarchitecture, and an additive manufacturing strategy working with shape memory and superelastic alloys will facilitate minimally invasive surgical procedures and sequential changes of geometries for unique metamorphic capabilities. These advantages will derive into a new generation of personalized and intelligent medical devices that will modify the status quo in cardiovascular surgery. The mentioned appliances, linked to high-performance active implants, will also open new horizons in the larger field of biomedical engineering, beyond cardiovascular applications. As for the future, the generated knowledge and developed geometries, materials and processes, will have a remarkable impact in different sectors including healthcare, transport, energy and space.

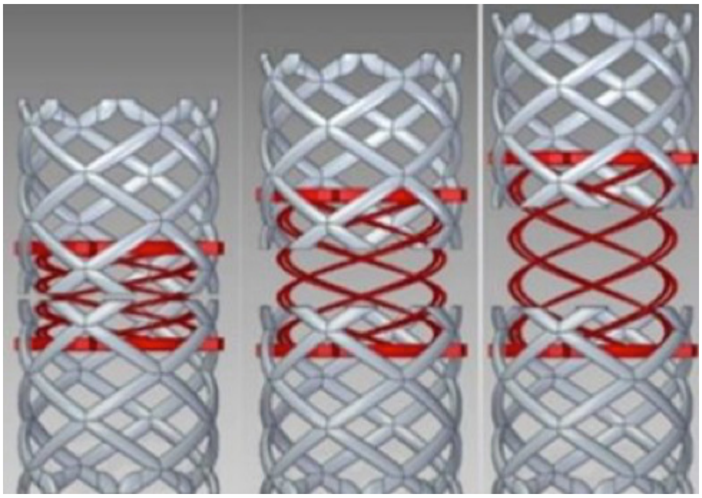


Figure 1: The concept of the implants to be developed under the i-MPLANTS-CM project

Research highlights

Bio-based phase change materials for thermal management

The development of thermal energy storage materials is the most attractive strategy to harvest solar energy, perform thermal management and increase energy utilization efficiency. Phase change materials (PCMs) have received much attention in this research field for several decades. Herein, IMDEA Materials has developed several new type biobased supramolecular phase change materials via molecular design and advanced synthesis [1-3], which have good potential to be applied in solar energy harvesting, thermal energy storage, wall insulation, smart windows, electrical devices, thermal management, artificial muscles, etc (Figure 1).

Going into more detail, the following approaches are being pursued in our Institute:

- A totally novel insight for polyrotaxane application and new design method for form-stable PCMs. Results shown that the mechanical performance, thermal stability in air and shape memory properties of polyrotaxanes are enhanced significantly compared to those of PEO. The form stability at temperatures above the melting point of PEO significantly increase with the α-CD addition. Polyrotaxane films are therefore promising sustainable and advanced form-stable PCM for thermal energy storage due to their high phase transition enthalpy and excellent

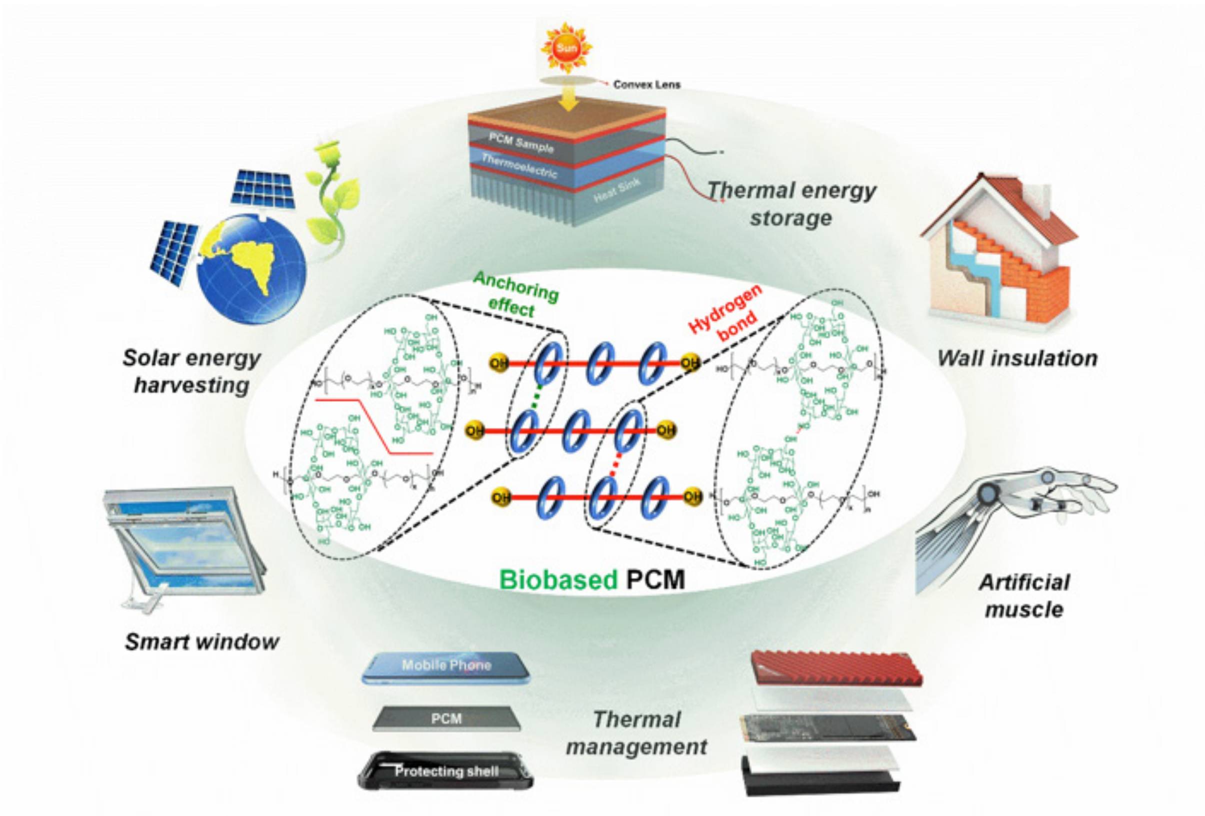


Figure 1. Polyrotaxane based supramolecular phase change materials: chemical structure and typical advanced applications.

cycle performance, Their ultra-high flexibility, remolding ability and excellent shape memory properties provide a convenient way for intelligent heat treatment packaging of complex and flexible electronic devices.

- A novel fully bio-based Poly (Glycerol-Itaconic acid) (PGI) was designed and synthesized with high efficiency by solvent-free polycondensation. Poly (ethylene glycol) (PEG) was used as the PCM working substance and was encapsulated by the sustainable PGI supporter. PEG chains were tightly encapsulated with the PGI supporting material mainly under hydrogen bonds due to the structural compatibility between PGI and PEG. The PCMs can achieve high form stability and high phase change enthalpies in the same kinds of PCMs. Furthermore, the phase change temperatures and enthalpies of the PCMs can be adjusted conveniently by regulating the PEG content and molecular weight. This process extremely facilitates their mass production due to the eco-friendly nature, high efficiency and low cost.

- A fire safe PCM was prepared by blending ammonium polyphosphate (APP) and poly (glycerol-itaconic acid) loaded polyethylene glycol (PEG). Results showed that limiting oxygen index (LOI) increased significantly with the increase of APP content. Typically, when the filling amount of APP reached 15 wt.%, the LOI value increased from 21.6% to 28.7%, vertical testing reached UL-94 V0 rating and the pHRR decreased by 36.15%. As-prepared PCMs show excellent form stability, and the enthalpy of phase change keeps higher than 70 J g-1, which is at the high level as that of same kinds of PCMs. These materials can be particularly useful for building thermal regulation due to their high preparation efficiency for PCM fabrication (and the profiles of all bio-based supporting matrix), the solvent-free pathway used, their mild curing temperature, and their fire safety.

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

[1] G-Z Yin, J. Hobson, Y. Duan, D-Y Wang, *Polyrotaxane: New generation of sustainable, ultra-flexible, form-stable and smart phase change materials.* **Energy Storage Materials 40**, 347-357 (2021).

[2] G-Z Yin, J. L. Díaz Palencia, D-Y Wang, *Fully bio-based Poly (Glycerol-Itaconic acid) as supporter for PEG based form stable phase change materials*, **Composites Communications 27**, 100893 (2021).

[3] G-Z Yin, X-M Yang, J Hobson, A. M. López, D-Y Wang, *Bio-based poly (glycerol-itaconic acid)/PEG/APP as form stable and efficiently flame-retardant phase change materials*, **Composites Communications 30**, 101057 (2022).

Preparation and characterization of supramolecular hydrogels based on a bis-urea derivative

Hydrogels can be formed from polymers or small molecules, from either natural or synthetic sources. Further, they can be classified by the types of bonds that form the hydrogel network – either covalent or non-covalent. Supramolecular hydrogels, particularly those formed from the non-covalent self-assembly of small molecule gelators, are relevant for biomedical applications because they have interesting properties. For example, some can be injected through a needle like a liquid and reform a solid structure, and they mimic the hydrated microenvironment of cells in the body. One such type of hydrogel that is often reported in the literature uses self-assembling peptides to form a nanofibrous network [1]. However, biocompatible hydrogels based on small molecule gelators that are not peptides are much rarer. A recently discovered novel supramolecular hydrogel based on a bis-urea derivative (<500 Da) has shown unexpectedly good results in supporting the viability and growth of cells [2]. Our group on Biomaterials and Regenerative Medicine is researching ways to improve these hydrogels in terms of mechanical properties and nanostructure. Our Institute also has state-of-the-art equipment to enable the characterization of the chemical, mechanical, and morphological properties of both the gelator compounds and the hydrogels [3] as well as new cell culture facilities to evaluate their cytocompatibility.

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

[1] M. EzEldeen, B. Toprakhisar, D. Murgia, N. Smisdom, O. Deschaume, C. Bartic, H. Van Oosterwyck, R. V. Sousa Pereira, G. Opdenakker, I. Lambrichts, A. Bronckaers, R. Jacobs, J. Patterson, *Chlorite oxidized oxyamylose differentially influences the microstructure of fibrin and self assembling peptide hydrogels as well as dental pulp stem cell behavior*, **Scientific Reports 11**, 5687 (2021).

[2] L. A. J. Rutgeerts, A. H. Soultan, R. Subramani, B. Toprakhisar, H. Ramon, M. C. Paderes, W. M. De Borggraeve, J. Patterson, *Robust scalable synthesis of a bis-urea derivative forming thixotropic and cytocompatible supramolecular hydrogels*, **Chemical Communications 51** (2019)

[3] B. Denzer, R. Kulchar, R. B. Huang, J. Patterson, *Advanced methods for the characterization of supramolecular hydrogels*. **Gels 7**, 158 (2021)

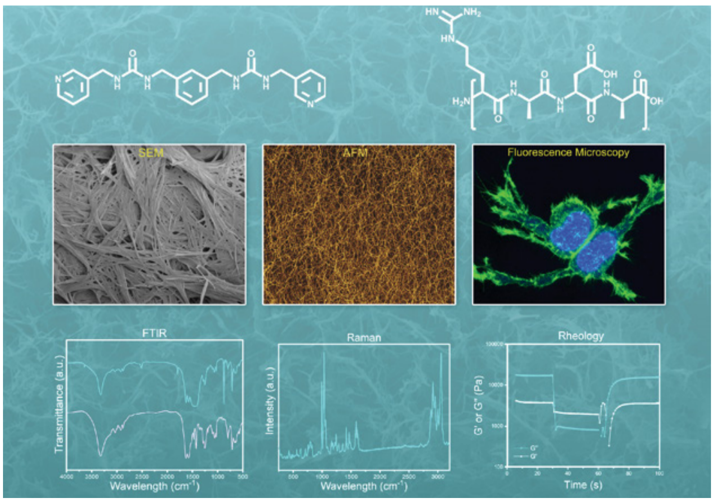
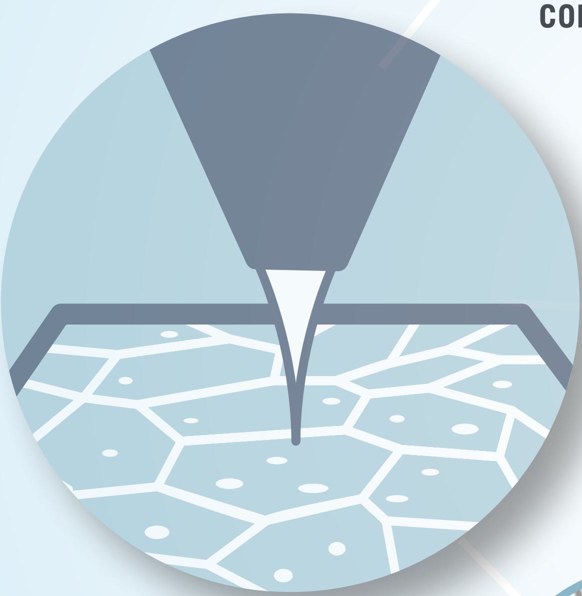


Figure 1. Synthesis and characterization of low molecular weight hydrogelators. (top row) Chemical structures of a bis-urea derivative and a self-assembling peptide capable of forming supramolecular hydrogels. (middle row and image background) Morphological characterization of representative hydrogels using scanning electron microscopy (SEM) and atomic force microscopy (AFM) as well as of cells growing within the hydrogels using confocal microscopy. (bottom row) Chemical and physical characterization of the hydrogelators and hydrogels using Fourier-transform infrared (FTIR) spectroscopy, Raman spectroscopy, and rheology (strain-recovery experiment).

programme
Advanced Manufacturing

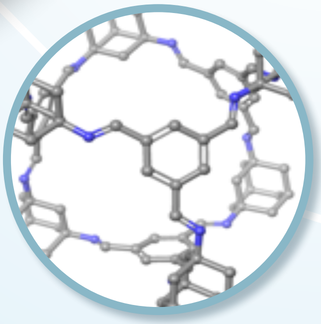
Structural composites



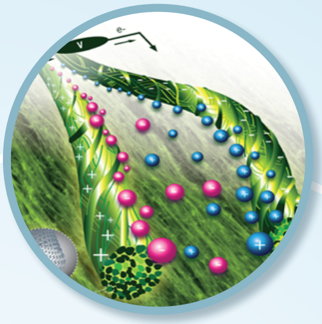
Goal and vision

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 realization of emerging products in the aerospace, biomedical, energy, automotive and other industrial sectors.

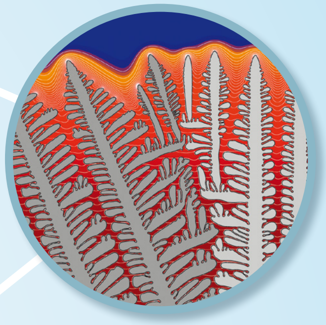
Effective unit-process innovation and development derives from an understanding of the physical and chemical phenomena influencing manufacturing processes. Therefore, a key part of this programme involves the creation and development of models based on Artificial Intelligence (AI) to predict the optimum 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 characterization techniques needed to monitor the quality of manufactured products including their (micro)structure and mechanical and functional properties.



Computational and Data-Driven Materials Discovery

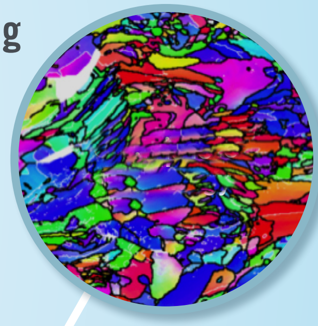


Multifuncional Nanocomposites

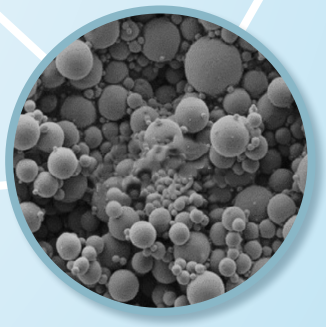


Modelling and Simulation of Materials Processing

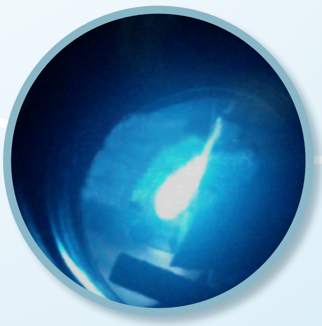
Physical Simulation



Sustainable Metallurgy



Sustainable Powder Metallurgy



Solidification Processing & Engineering

Main research lines

Industry 4.0

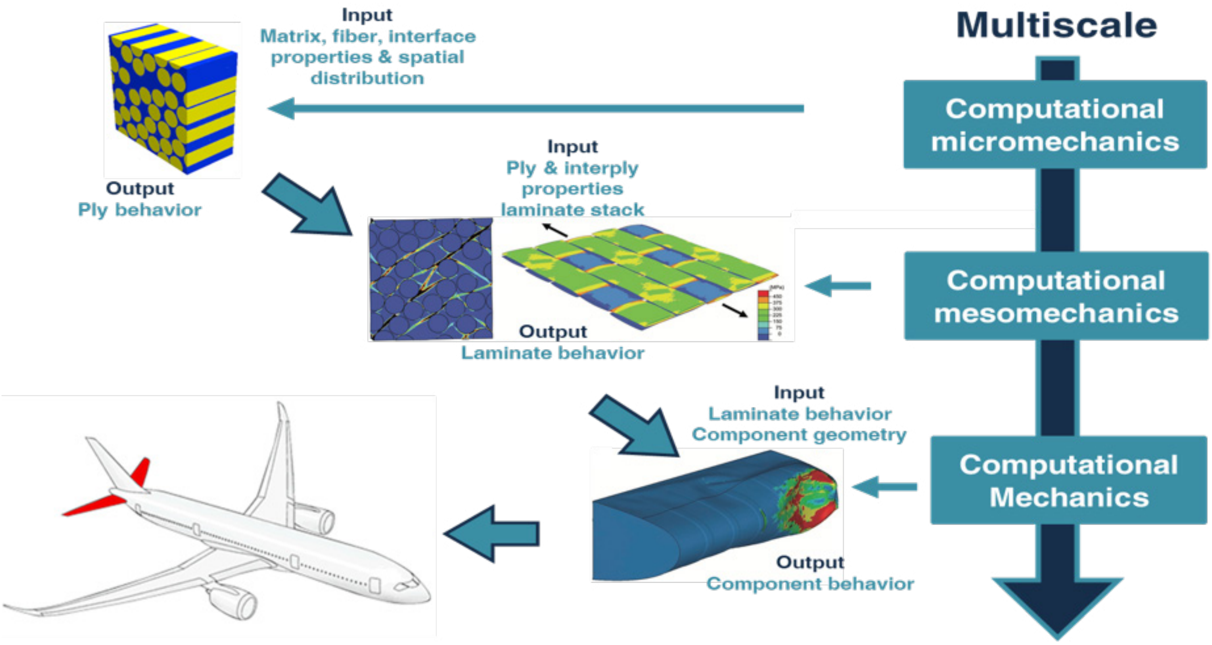
- Virtual testing of structural composites. Analysis of the effect of manufacturing defects on structural performance.
- Virtual processing of structural composites including hot-forming and out-of-autoclave (injection, infusion, compression moulding). Surrogate and reduced order models for manufacturing 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

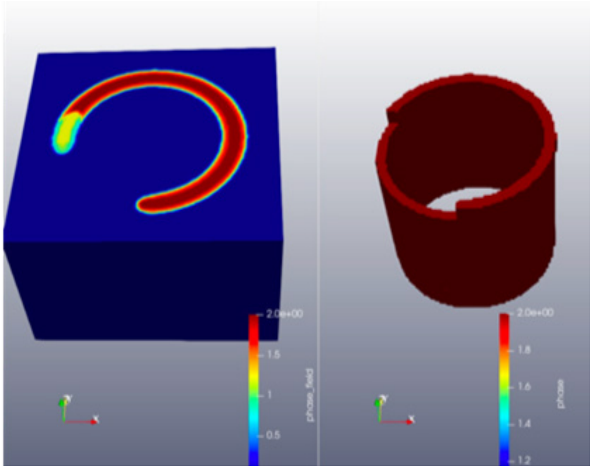
- Gas-phase assembly of continuous fabrics and fibres of carbon nanotubes and inorganic nanowires (Si, SiC).
- Integration of these nanostructured fabrics into electrochemical devices and composite materials.

Liquid and solid-state processing

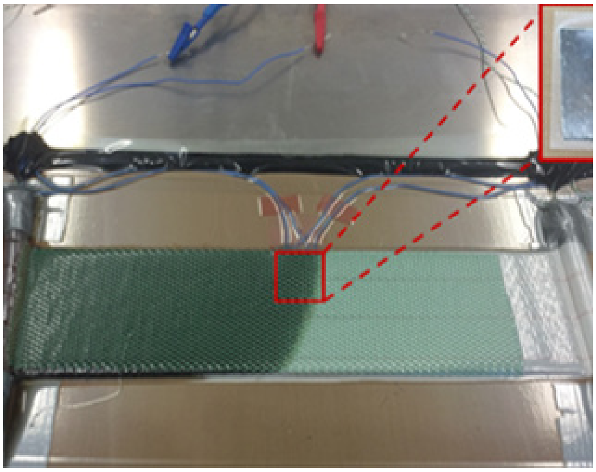
- Rapid alloy prototyping and manufacturing of bulk alloy libraries for the fast assessment of properties.
- Optimisation of casting processes.



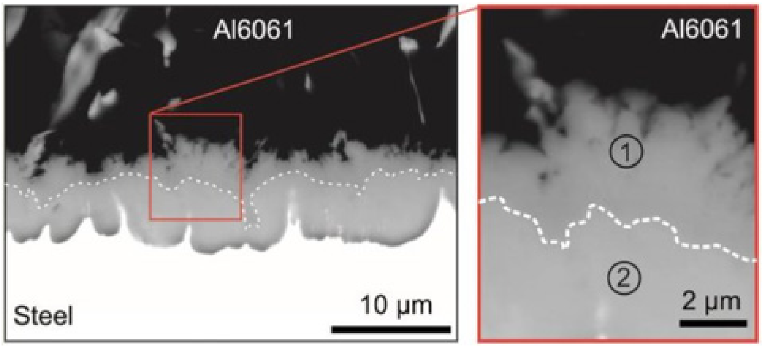
Virtual testing strategy for composites (static and dynamic properties)



Finite element modelling of selective laser melting processing. Temperature (left) and layer-by-layer addition of materials by selective melting (right)



Structural supercapacitor produced by stamping a carbon nanotube fibre-based electric double-layer capacitor (EDLC) interleaf, embedding it between carbon fibre plies and infusion/curing of epoxy resin



Physical simulation of joining of dissimilar materials, steel and aluminium) to predict the interface and its properties.

- Development of novel thermo-mechanical processes and powder metallurgy routes via mechanical alloying and gas atomization in non-oxidation conditions.
- Consolidation by field-assisted sintering and conventional press and sintering.

3D printing

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

Projects in focus

DOMMINIO / Digital method for improved manufacturing of next-generation multIfunctIonal airframe parts

Funding: European Commission/Horizon 2020 Programme - Societal Challenges - Smart, Green and Integrated Transport
Partners: AIMEN (Coordinator), IMDEA Materials Institute, National Technical University of Athens, Ecole Nationale Superieure d'arts et Metiers, industrial technical center for lastics and composites, INCAS, Tortech Nano Fibers, Dasel sistemas, Innovation in research & engineering solutions, EASN, BAE systems, ESI group and Aciturri Engineering
Project period: 2021 - 2024
Principal Investigators: Dr. J. J. Vilatela and Prof. C. González

In the last few decades, the aeronautical industry has experienced a drastic transformation in the manufacturing philosophy in response to the growth of aircraft production (by 60% in the last 10 years). At the same time, there is a transition to the usage of advanced composite materials, due to their lightweight properties, strength and durability. The use of such novel advanced materials together with the increased aircraft productivity and performance increase the challenges in the design and manufacturing of cost-effective aircraft structures and components, allowing weight and fuel consumption reduction, shorter manufacturing cycles and increased energy efficiency in aircraft fabrication.

The DOMMINIO project will develop an innovative methodology to ensure cost-effective, efficient and sustainable manufacturing of high quality multifunctional and intelligent airframe parts based on (see the project concept in Figure 1):

- Robotized technologies (ATL, FFF)
- Advanced simulation tools
- Online process & quality monitoring
- SHM (Structural Health monitoring) methods enabled by real-time data-driven fault detection

In particular, the project objectives are:

- Enable flexible multistage robotic-based production processes for manufacturing of multifunctional composite airframe parts
- Develop novel data-driven pipeline supporting the design, simulation and production planning of multifunctional and intelligent composite airframe components
- Develop a Quality-by-Design (QbD) manufacturing strategy, based on the development of process control and advanced quality monitoring systems
- Develop a new digital-combined-physical driven methodology for monitoring and managing the health of multifunctional airframe parts.

Achieving these objectives will produce the following impacts:

- To reduce by 25% the manufacturing costs of additive manufacturing technologies
- To decrease 25% the design time (product & process)
- To reduce component weight by 20%
- To reduce maintenance, repair, and operations costs by 30%
- To reduce scrap by 15% and energy consumption by 10%

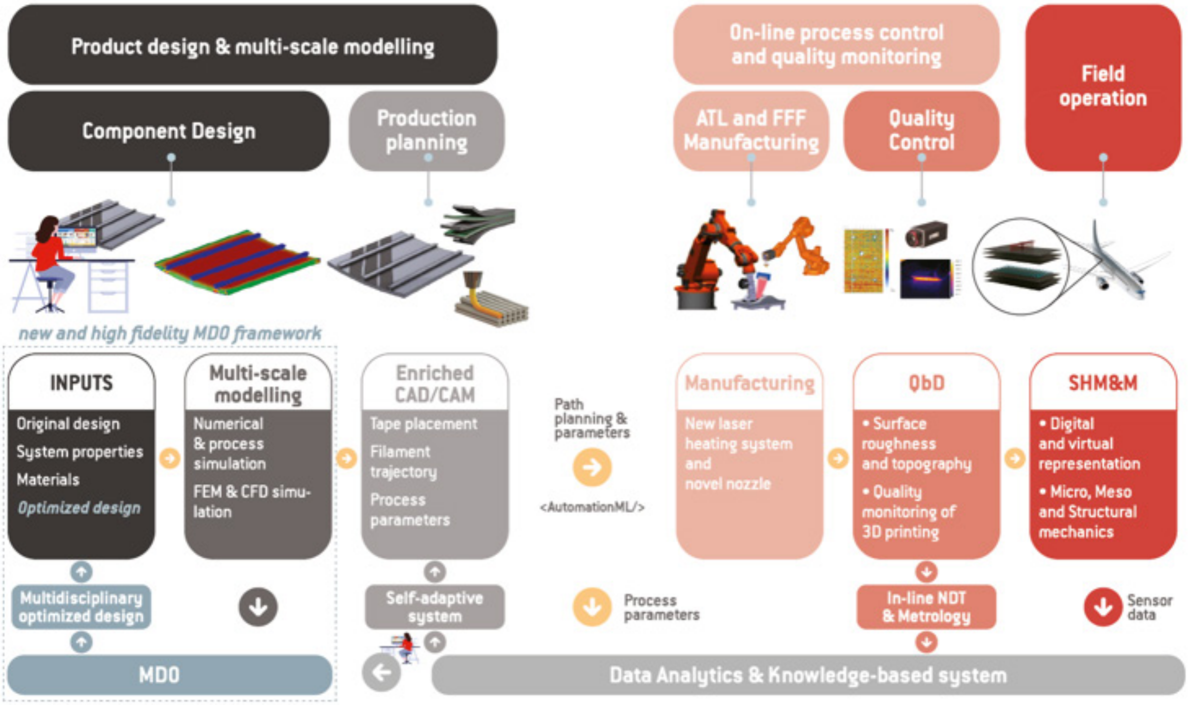


Figure 1. the concept of the DOMMINIO project.

IMDEA Materials activities within the DOMMINIO project will focus on the following two aspects:

- The fabrication and modification of carbon nanotube (CNT) fibres for integration in multifunctional composites. Our involvement will be from the material specifications, filament developments and functionalities evaluation up to advisory tasks for scale-up production by Tortech Nano Fibers.
- The development of digital twins and virtual testing tools for the SHM analysis of structural composites. Virtual testing tools will be developed to simulate the mechanical behaviour of laminates containing CNT fibres produced by AIMEN at the micro, meso and laminate level. The SHM will be based on a deep learning model trained with numerical results with the purpose of ascertaining the position of artificial damages introduced in a panel from the CNT strain signals.

Additive manufacturing of Aluminium alloys

Additive Manufacturing (AM), or 3D printing of metals, one of the key technologies powering the industry 4.0 revolution, allows for a significant reduction in weight, freedom of design, component customization, cutback of lead time facilitated by in-house production, and decreased waste. As such, AM is shifting the basis for competition in the fabrication of medical implants and aeronautical components, among others, thus disrupting traditional supply chains.

However, the number of metallic materials that can be processed by AM into components with a robust structural behavior is still rather limited. In particular, among the commercial aluminum alloys, only the low performance AlSi casting system, including AlSi7Mg, AlSi10Mg, and AlSi12, can be reliably printed. The high strength age-hardenable aluminium alloys belonging to the 7xxx and 2xxx series can in general not be efficiently processed by AM as the non-equilibrium melting and solidification processes involved often result in undesirable microstructures with large columnar grains and with a propensity for cracking. In addition, during AM processing under vacuum conditions, common alloying elements such as Zn, Mg, and Li, which form the age hardening phases, are highly volatile and evaporate preferentially, thus decreasing their high precipitation strengthening potential. Other challenges associated to the additive manufacturing of Al alloys are the high reflectivity of the aluminium powder as well as its high reactivity with oxygen, which leads to the growth of surface oxide films that give rise to an increased density of defects in the printed samples. The high demand for lightweighting of structural and engine components in transportation vehicles, triggered by the urgent need to reduce energy consumption and CO_2 emissions, requires developing new aluminium alloy systems with high thermal stability and improved strength at a wide range of temperatures, and which are printable and affordable.

IMDEA Materials Institute is working on the development of Al alloys that are specifically tailored for additive manufacturing and, in particular, for selective laser melting. The following approaches are being pursued in order to achieve that goal:

- Alteration of the composition of traditional alloys by the addition of grain refiners, such as Zr, both as alloying element as well as via mixing with microparticles [1].

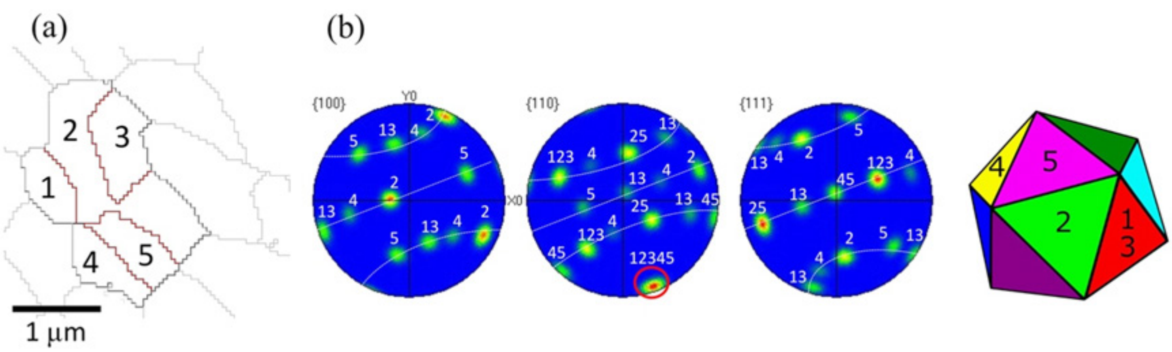


Figure 1. (a) Cluster of grains in a 7075 alloy resulting from nucleation on an icosahedral quasicrystalline template during selective laser melting; (b) Direct pole figures illustrating the orientation relationships between the grains in (a) and icosahedral quasicrystal template, indicating the growth faces corresponding to each grain [2].

- Enhancement of grain refinement by the stimulation of alternative, and rare, solidification mechanisms, such as icosahedral quasicrystal enhanced nucleation (Figure 1) [2].

- Revisiting rapid solidification alloys, including low diffusivity transition elements, where quasicrystal formation during processing ensures unprecedented thermal stability.

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[1] A. Martín, M. San Sebastián, E. Gil, C.Y. Wang, S. Milenkovic, M.T. Pérez-Prado, C.M. Cepeda-Jiménez, *Effect of the heat treatment on the microstructure and hardness evolution of an AlSi10MgCu alloy designed for laser powder bed fusion*, **Materials Science and Engineering A 819**, 141487 (2021)

[2] C. Galera-Rueda, M. Montero-Sistiaga, K. Vanmeensel, M. Godino-Martínez, J. LLorca, M.T. Pérez-Prado, *Icosahedral quasicrystal enhanced nucleation in Al alloys fabricated by selective laser melting*, **Additive Manufacturing 44**, 102053 (2021)

Advanced high entropy alloys

High entropy alloys (HEAs) have been postulated as candidates to replace conventional alloys because of their good combination of properties such as high microstructural stability, good mechanical properties, and resistance to oxidation and corrosion. The high entropy (HE) concept has introduced a new criterion in the design of alloys that opens a variety of design considerations not only in the domain of HEAs but also in other families of alloys, such as the high entropy superalloys (HESAs). At IMDEA Materials Institute, multiple research initiatives are undertaken to design and develop novel HEAs and HESAs based on the framework of sustainable metallurgy. Some researches that are currently active are summarized as follows:

1) In the MAT4.0-CM project, a new family of HEAs was developed based on solid-solution formation rules, segregation parameter (λ), and thermodynamic calculations by addition of Cu, Mo, and/or the combination of both elements up to 10 at. % into $CoCrFe_2Ni_2$ system. These alloys showed a single FCC phase once the microstructure was homogenized at 1200 °C. It was also demonstrated that the Cu-Mo interaction is responsible for inhibiting or delaying the precipitation of both Cu-rich and Mo-rich particles and the maintenance of a single FCC crystal.

2) Even though ingot metallurgy has been considered the most commonly used method to manufacture HEAs, powder metallurgy (PM) offers better microstructure control and new processing methods like additive manufacturing (AM), particularly Selective laser melting (SLM) to develop a wide range of HEAs. Since HEAs involve at least five elements in near-equal quantities, they are expensive to manufacture particularly for sustainable manufacturing technologies. So, we are introducing new economical, time and energy-saving, and environmentally friendly approaches for developing fully PM-based HEAs and available feedstocks for additively manufactured components which also makes it a viable option for industrial implementation [1]. Our aim is to develop competitive HEAs that can compete with/exceed the mechanical properties of conventional Ni superalloys at high temperatures. Instead of starting with pure elemental powders or fully pre-alloyed powders, we use commercial commodity powders already available on the market like stainless steel, Ni and Co-based superalloys, etc. They are

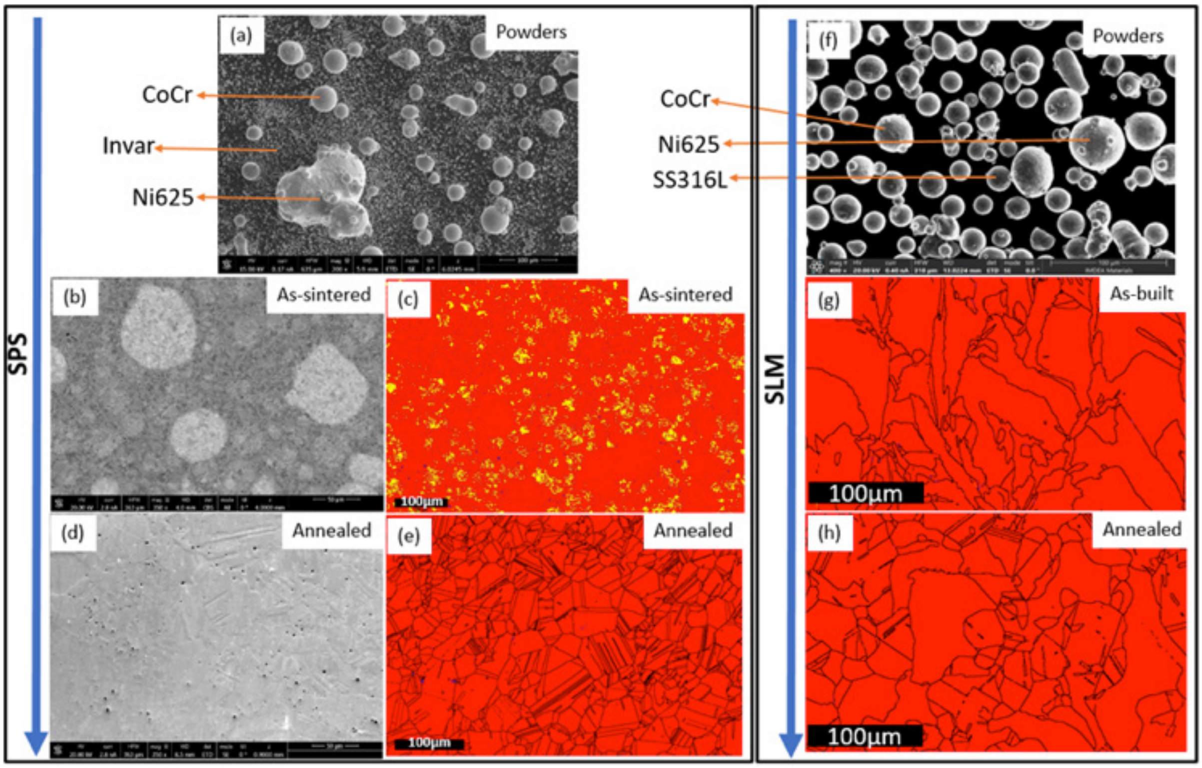

Figure 1. (a)-(e) Spark plasma sinter (SPS) process, (f)-(h) Selective laser melting (SLM) process. (a) shows the powders used for SPS, (b) and (c) show the SEM image and EBSD phase map respectively of the as-sintered samples sintered at 1000 ºC, (d) and (e) show the SEM image and EBSD phase map respectively of the same samples annealed at 1200 ºC for 24 hours. (f) shows the powders used for SLM, (g) shows the EBSD phase map of the as-built sample consisting of columnar grains, and (h) shows the same sample annealed at 1200 ºC for 4 hours where the grains are equi-axial.

relatively cheaper and are industrially available in a wide range of size distributions and morphologies. The most intriguing part of this research is how the diffusion of different elements during annealing gives rise to a single FCC phase and also leads to a homogenous distribution of elements as shown in Figure 1.

3) The HE criterion can be applied to develop new Co-based superalloys, strengthened by λλprecipitates, with improved high-temperature performance. However, the production of Co-based superalloys via advanced sustainable manufacturing processes has several issues. CNSTech project proposes the development of the next generation PM-based CoNi high entropy superalloys via a sustainable metallurgy framework [2]. In the pre-build design step of this work, the aim is to develop an accelerated approach using the CALPHAD method and high entropy alloys concept to achieve a CoNi based high entropy superalloy. Figure 2 shows a high entropy FCC matrix that contains λand λλphases successfully produced concomitantly with the formation of the B2 phase in an arc melted alloy after the homogenization.

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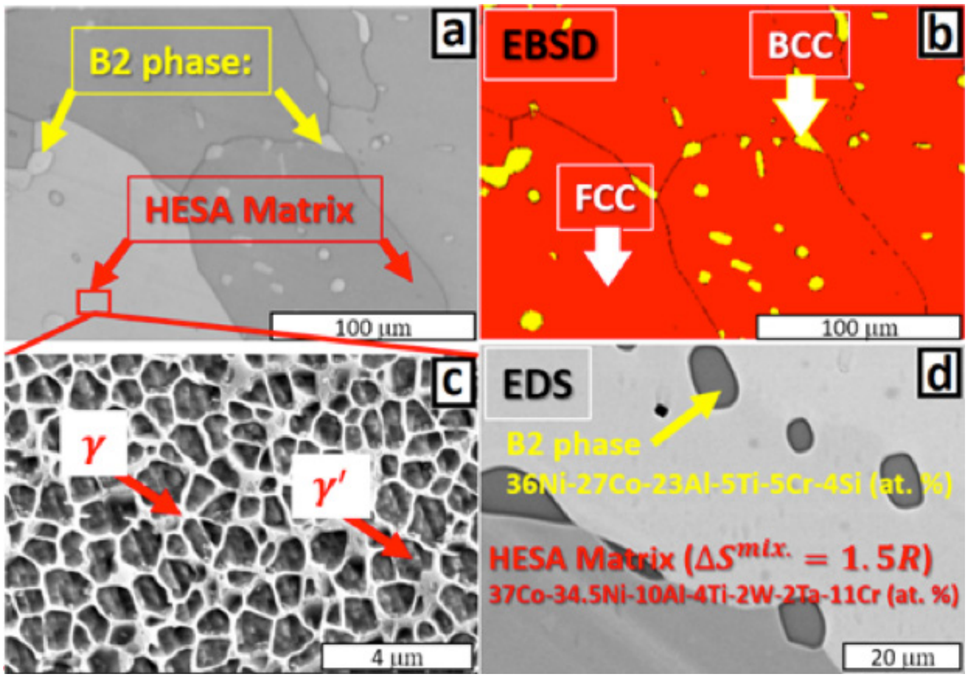


Figure 2. a) SEM image, b) EBSD phase map, c) FESEM image of the γ and γ' phases, and d) EDS analysis of a CoNi based HESA homogenized alloy at 1200 °C for 24 h.

[1] I. Toda-Caraballo, J. A. Jiménez, S. Milenkovic, J. Jimenez-Aguirre, D. San-Martin, *Microstructural Stability of the CoCrFe2Ni2 High Entropy Alloys with Additions of Cu and Mo*, **Metals 11**, 1994 (2021)

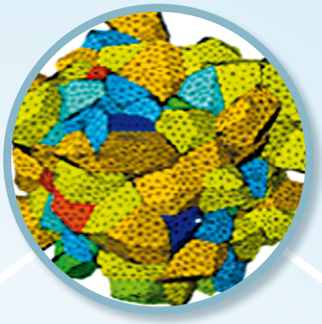
[2] J. M. Torralba, S. Venkatesh Kumaran, *Development of competitive high-entropy alloys using commodity powders*, **Materials Letters 301**, 130202. (2021)

programme

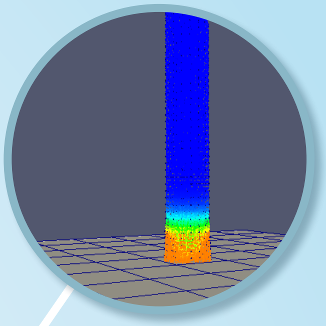
Integrated Computational Materials Engineering

Goal and vision

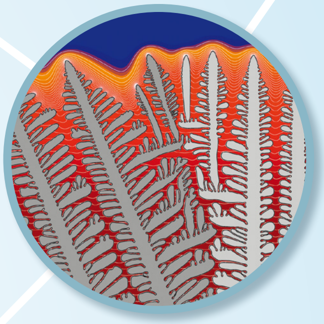
The research programme on Integrated Computational Materials Engineering (ICME) is aimed at integrating all the available simulation tools into multiscale modelling strategies capable of simulating processing, microstructure, properties and performance of engineering materials, so new materials can be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



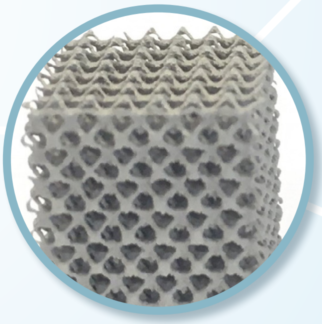
Multiscale Materials Modelling



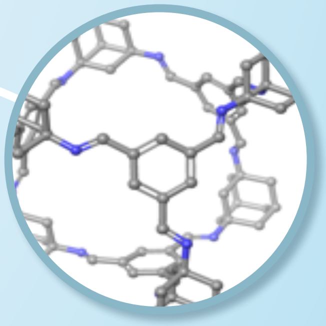
Computational Solid Mechanics



Modelling and Simulation of Materials Processing



Bio/Chemo/Mechanics of Materials



Computational and Data-Driven Materials Discovery

Main research lines

Virtual materials design, including virtual processing and virtual testing

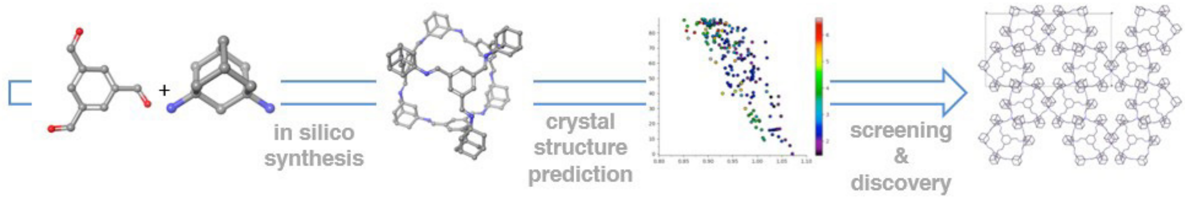
- Virtual material discovery for functional applications, through the use of DFT, cluster expansion and atomistic approaches combined with AI.
- Virtual processing: Integration of modelling tools (atomistic, computational thermodynamics and kinetics, phase-field) to simulate the microstructural development of materials during processing.
- Virtual testing of metallic alloys: Development, calibration and numerical implementation 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 polycrystalline homogenization.
- 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
  - Light (Al, Mg and Ti) metallic alloys and their composites.
  - Ni-based superalloys.
  - 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 computational homogenization.

Multiscale materials modelling

- Bottom-up approaches (scale bridging).
- Development of modular multi-scale tools.
- High throughput screening integration.
- Concurrent models.
- Mean-field homogenisation
- Computational homogenization including FEM and Fast Fourier Transform –FFT–based solvers
- Modelling and simulation of multiscale transport phenomena (application to advanced materials for batteries).



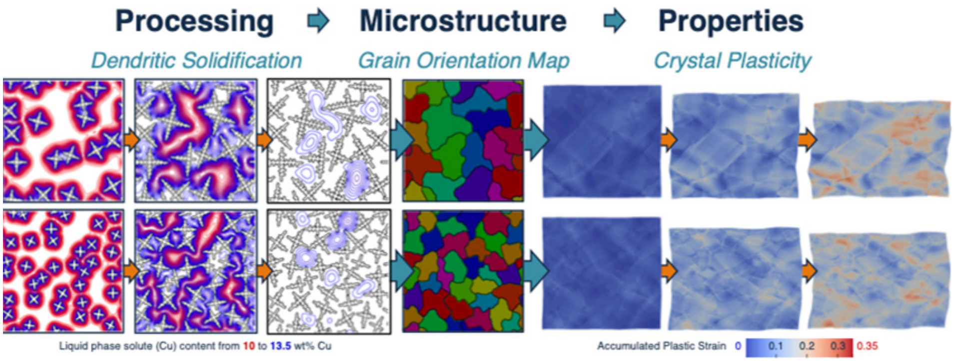
Computational, data-driven materials discovery

Modelling and simulation strategies for different applications

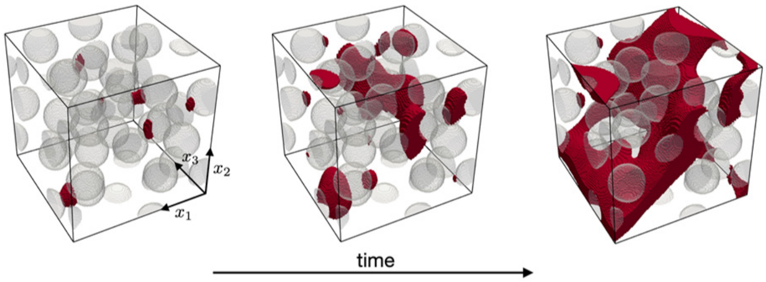
- Multiscale modelling of dendritic growth (dendritic needle network approach).
- Numerical methods for solids (finite elements and FFT approaches).
- Computational mechanics and micromechanics.
- Material informatics for analysis of large material datasets.
- Modelling and simulation of H_2 embrittlement 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.
- Virtual design and testing of mechanical metamaterials.
- Simulation of the additive manufacturing process in metals including macroscopic simulation of the thermo-mechanical process by multiphysics finite element models, microstructure evolution through phase-field and prediction of mechanical response using computational polycrystalline homogenization.

Computational and data-driven materials discovery

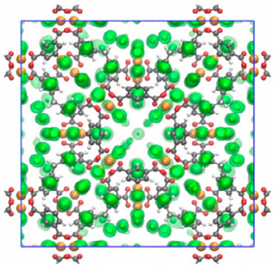
- Discovery of porous materials for energy applications (CO_2 capture, methane storage).
- Design of ionic liquids.
- Materials discovery: structures with high H_2 working capacity and H_2 adsorption-desorption performance.
- Porous material design for capture and storage of CO_2.
- Design of Metal-Organic 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



Ductile failure at the microscale using FFT and non-local models



Predicted distribution of Xe atoms in MOF

Projects in focus

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

Funding: Institution/Programme: Spanish Ministry of Science and Innovation/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Collaboration Challenges
Partners: ITP Aero (Coordinator), Technical University of Madrid, University of the Basque Country, IMDEA Materials Institute
Project period: 2018 – 2021
Principal Investigators: Prof. I. Romero, Prof. J. Segurado and Dr. D. Tourret

The ENVIDIA project (*Virtual environment for the design and manufacturing of airplane turbine*) has contributed to the development of predictive simulation capabilities for the design of the next generation of aircraft turbines. In this collaborative project, coordinated by world-leading aeroengine manufacturer ITP Aero, the role of IMDEA Materials Institute focused on linking processing, microstructures, and properties of Nickel-based superalloys produced by additive manufacturing (Laser Powder Bed Fusion, LPBF). In order to progress toward a fully integrated software solution for alloy design and process optimization (Figure 1), IMDEA Materials has developed new simulation tools along two main directions: (1) multiscale thermo-mechanics and microstructure formation models during LPBF, in order to link processing and microstructures, and (2) micro-mechanical modelling of heterogeneous microstructures, in order to link microstructures to mechanical properties and performance.

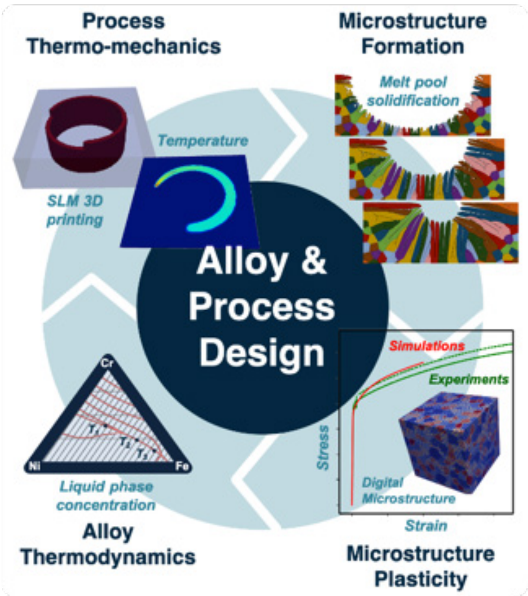


Figure 1. Integrated computational framework for LPBF of metallic alloys.

Linking processing to microstructures

Our Institute has developed a multi-scale simulations framework (Figure 2), which integrates: (i) a finite element (FE) thermo-mechanical model to predict residual stresses and temperature profile and history during LPBF, (ii) a phase-field (PF) model of microstructure formation in the melt pool, and (iii) computational thermodynamics (CalPhaD) calculations of complex alloys properties. Thermo-mechanical simulations of LPBF are implemented in proprietary FE code IRIS with a computationally efficient representation of the powder bed as a continuum combining thermophysical properties of powder and surrounding gas and powder bed descriptors (e.g. packing fraction, particle sizes), and allows arbitrary laser path via a G-code interpreter (Figure 3). The microstructure formation PF model uses the temperature field from FE simulations to simulate the grain growth at the entire melt pool scale while retaining its accuracy at the level of individual dendrites/cells, using an in-house code massively parallelized on Graphics Processing Units (GPUs). CalPhaD calculations, using software ThermoCalc®, provide temperature-dependent thermophysical properties (e.g. heat capacity, density) and phase diagram features (e.g. phase

transformation temperatures, solubilities) used in FE and PF simulations, which allows exploring the effects of complex alloy chemistries at the level of the process and that of the microstructure [1].

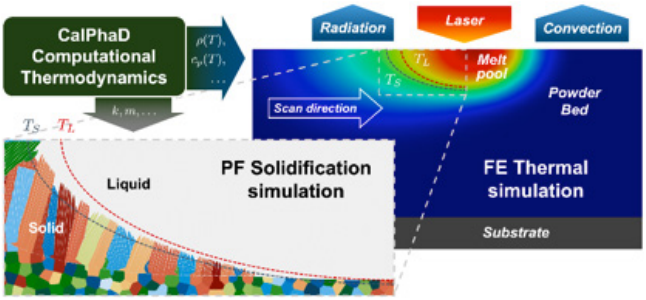


Figure 2. Integrated modeling framework for LPBF of metal alloys.

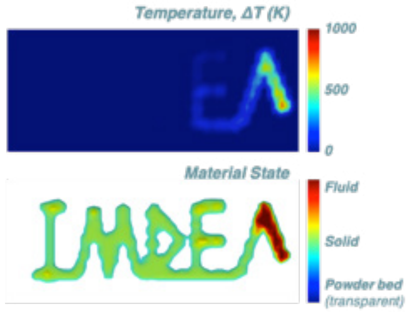


Figure 3. Arbitrary laser path.

Linking microstructures to properties and performance

IMDEA Materials used computational homogenization and crystal plasticity theory to predict the temperature-dependent response of Hastelloy-X superalloy in LPBF-printed parts, in order to study the heterogeneous and anisotropic mechanical response observed experimentally. Simulations were performed on Representative Volume Elements (RVEs) statistically representative of the grain size, shape, and orientation distributions measured experimentally for different printing directions and part thicknesses (Figure 4), using IMDEA Materials' proprietary homogenization code based on a computationally efficient Fast Fourier Transform formalism (FFTMAD). The model accurately predicts mechanical properties (e.g. Young's modulus, plastic stress–strain curves) of different specimens across a wide temperature range (Figure 5), and thus allowed to demonstrate the crucial effect of texture and grain aspect ratios induced by LPBF processing on the properties of printed parts [2].

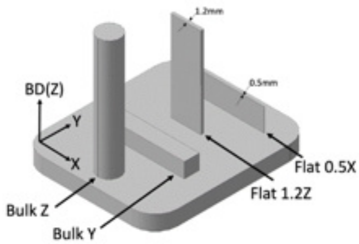


Figure 4. Printed specimens of different build directions and thicknesses.

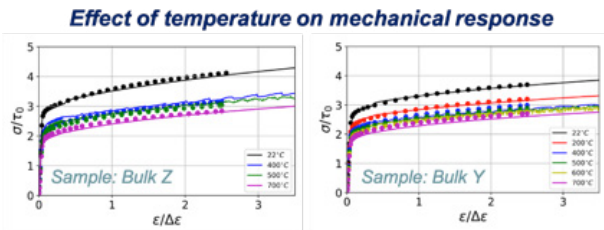


Figure 5. Temperature-dependent uniaxial stress–strain for different printed (symbols: simulations; solid lines: experiments).

Perspectives

By providing computational models to support – or substitute – the experimental trial-and-error innovation process, the outcome of the ENVIDIA project should accelerate the design of novel high-temperature alloys and the optimization of LPBF processing conditions and geometries, in order achieved unprecedented performance and durability in high-temperature applications.

[1] S.M. Elahi, R. Tavakoli, A.K.Boukellal, T. Isensee, I. Romero, D.Tourret, *Multiscale simulation of powder-bed fusion processing of metallic alloys*, **Computational Materials Science 209** 111383 (2022).

[2] C.M. Pilgar, A. M. Fernandez, S. Lucarini, J. Segurado, *Effect of printing direction and thickness on the mechanical behavior of SLM fabricated Hastelloy-X*, **International Journal of Plasticity 153** 103250 (2022).

Research highlights

Data-driven design of animal feed additives

The growing world population and its impact on the environment requires advanced agriculture technologies and products. Mycotoxin detoxifiers (MDTs) are an example of such additives. Mycotoxins are toxic secondary metabolites typically produced by fungi growing in food and animal feed commodities, and exposure to these contaminants may result in animal death or disease. The maximum levels of some of the most highly prevalent mycotoxins in animal feed are already controlled via guidance values or recommendations, rendering the need for mitigation strategies, such as mycotoxin capture by detoxifier feed additives, e.g. porous materials with high adsorption selectivity towards toxins. The global market for such products is growing and is expected to reach a ca value of USD 3.1 billion by 2027.

The development of food and feed additives involves the design of materials with specific properties that enable the desired function while minimizing the adverse effects of their interference with the concurrent complex biochemistry of the living organisms. Often, the development process is heavily dependent on costly and time-consuming in vitro and in vivo experiments. IMDEA Materials' researchers presented an alternative approach to design clay-based composite materials for mycotoxin removal from animal feed at a fraction of the current cost [1]. The approach can accommodate various material compositions and different toxin molecules. Using machine learning trained on in vitro results of mycotoxin adsorption-desorption in the gastrointestinal tract, we searched the space of possible composite material compositions to identify formulations with high removal capacity, gaining insights into their mode of action (Figure 1).

An in vivo toxicokinetic study, based on detecting biomarkers for mycotoxin exposure in broilers, validated

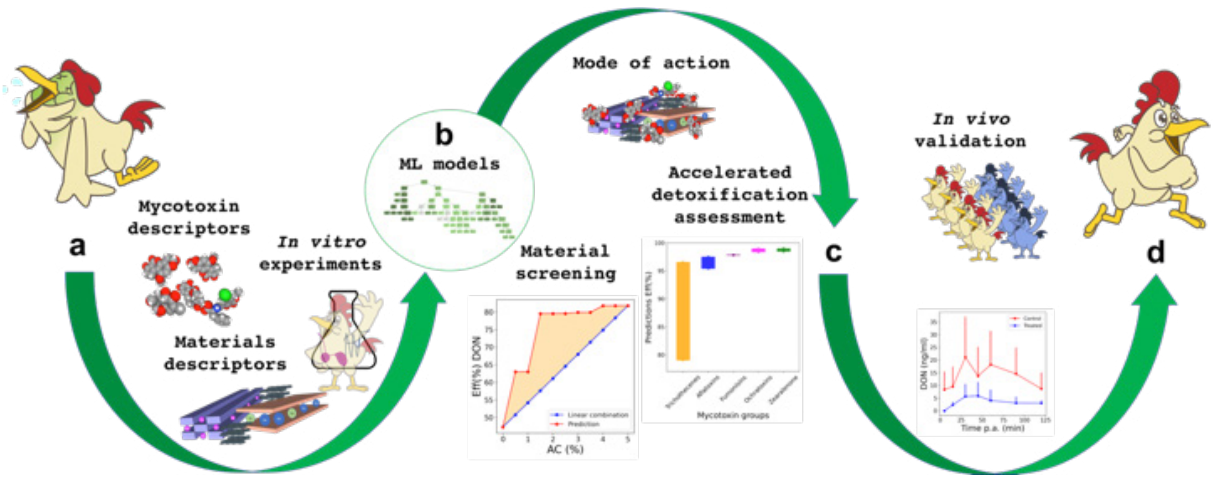


Figure 1. Workflow representation starting from selection of feature vector space (a) which describes the in vitro adsorption and efficiency (model targets). Machine learning models (b) trained on in vitro dataset providing tools for material screening, wide in vitro detoxification assessment, and mode of action capturing (c). In vivo validation of the findings extracted by our approach (d).

the findings by observing a significant reduction in systemic exposure to the challenging to be removed mycotoxin (i.e., deoxynivalenol (DON)) when the optimal detoxifier is administrated to the animals. For example, a mean reduction of 32% in the area under the plasma concentration-time curve of DON-sulphate was observed in the DON+detoxifier group compared to the DON group

For more information, please contact:
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[1] G. Lo Dico, S. Croubels, V. Carcelén, Maciej Haranczyk, *Machine learning-aided design of composite mycotoxin detoxifier material for animal feed*, **Scientific Reports 12**, 4838 (2022)

Artificial intelligence applied to the manufacturing of advanced materials

Promoting the efficient use of materials starting from their early design to the manufacturing and service life will increase overall system efficiency while reducing the environmental footprint. Even today, the burden of the cost of not producing optimum at right-first-time is enormous in terms of scraps, energy consumption, lost production and rework. With that in mind, the cumulative and recurrent costs for the non-implementation of the appropriate diagnosis manufacturing policies that could allow recovery from failure will undoubtedly negatively impact industry competitiveness. The classical

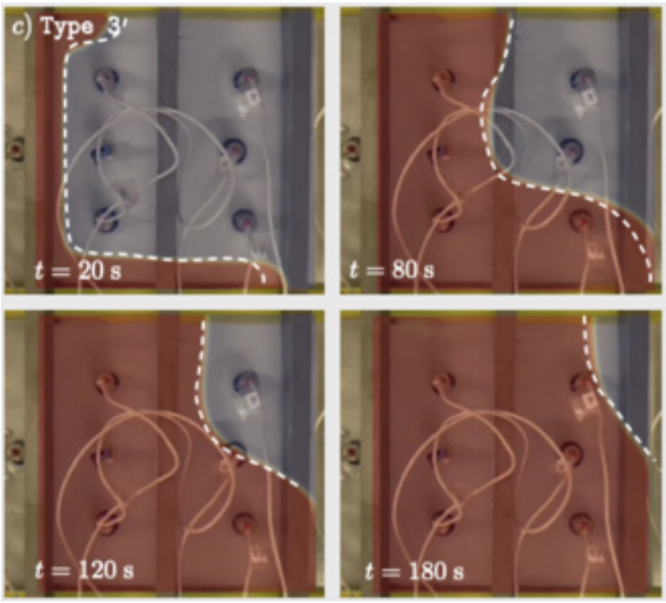

Figure 1. Flow front evolution for resin injection manufacturing process (red=impregnated material, grey=dry material). The AI ResNet system reads information from a set of pressure sensors distributed, classifying the problem and providing regression of the strength of the manufacturing disturbance, which is followed by a prediction of the front flow evolution (dotted lines).

phenomenological approach to design and manufacturing materials guided by trial-and-error gives way to a new paradigm in which material science and computational modelling evolve in a seamless hybridization with Artificial Intelligence (AI). IMDEA Materials is currently working on different approaches to incorporate AI into manufacturing lines for structural composites progressively:

Automated detection of processing disturbances during manufacturing of composite materials by Resin Transfer Moulding (RTM) [1]. Models were developed to address the problem of race-tracking regions (fast flow resin channels in Figure 1) and regions with dissimilar permeability. The detection capabilities of the models fall on the analysis of pressure changes recorded by a distributed network of sensors. The sensor readings are automatically analyzed using ResNet (Residual Network), which was already trained with synthetic data generated by finite volume simulations (OpenFoam). The deep learning network was used first to classify the type of processing disturbance (e.g. type of race-tracking) and, secondly, to measure its strength by regression of the basic parameters (e.g. length of the race-tracking channels).

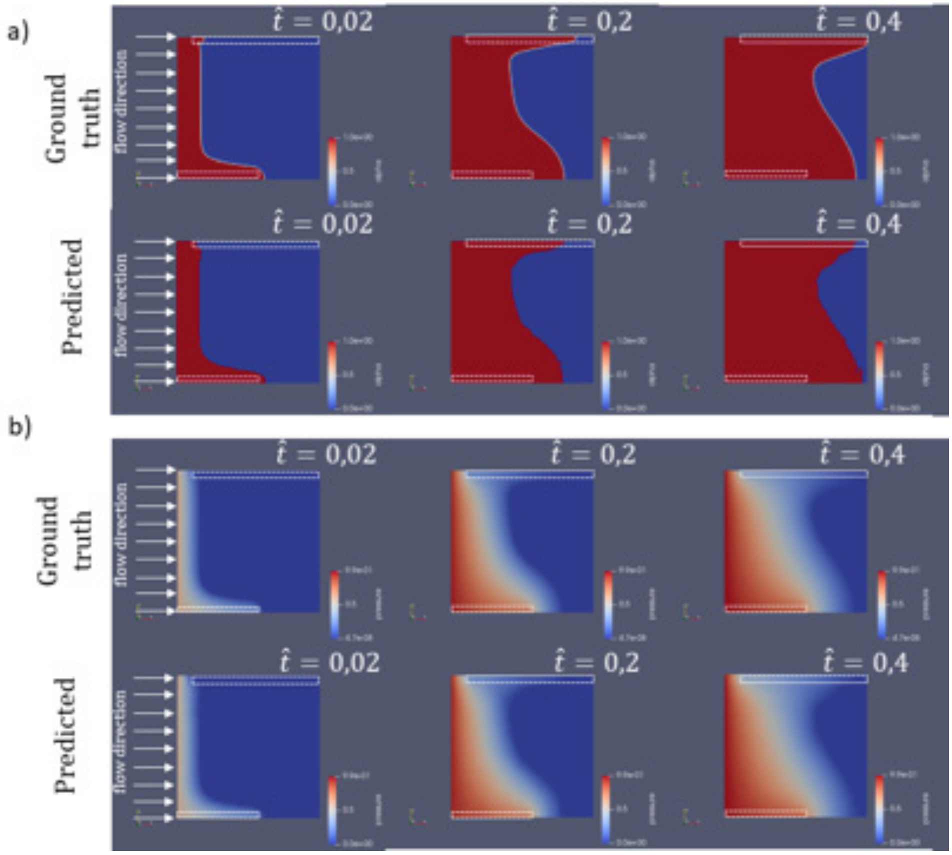

Figure 2. Comparison between surrogate deep learning model results for race-tracking and the corresponding ground truth values. The deep-learning encoder-decoder reads the boundary conditions of the problem and provides simulations results (pressure and flow front fields) almost instantaneously.

Surrogate modelling [2]. Today, one of the more severe bottlenecks in simulation for optimizing material processing is the impossibility of getting a prompt and proper response in real-time. Surrogates will enable the generation of digital twins for processing that can be deployed at the factory level. IMDEA Materials is developing surrogates for RTM manufacturing using deep-learning encoder-decoder architectures, trained with synthetic data generated by finite volume simulations. The deep-learning structure encodes the inputs of the problem (e.g. geometry, boundary conditions) into a minimum latent variable space which is then followed by an expansion into the entire synthetic fields (e.g. pressure and flow front). Once trained, the encoder-decoder can instantly deliver pressure and front flow fields given the boundary conditions. Therefore, deployment at the industrial floor level is affordable. Figure 2 shows the pressure and front flow evolution snap-shots during the resin filling of an RTM mould. The ground truth obtained with the finite volume simulations with OpenFoam is compared with the deep learning encoder-decoder's predictions.

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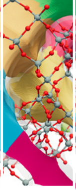
[1] J. Fernández-León, K. Keramati, D. Garoz, L. Baumela, C. Giraldo, C. González, *A machine learning strategy for race-tracking detection during manufacturing of composites by liquid moulding*, **Integrating Materials and Manufacturing Innovation**, in the press (2022).

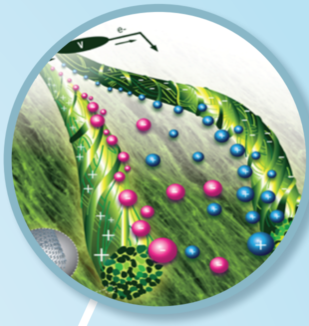
[2] J. Fernández-León, L. Baumela, C. González, *A Deep Encoder-Decoder neural network for surrogate modelling of liquid moulding of composites*, submitted for publication (2022).



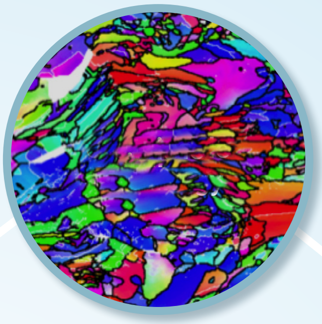
programme Multiscale Characterisation of Materials and Processes

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.



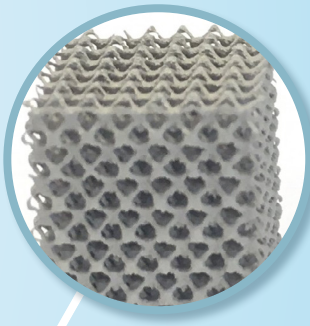
Multifunctional Nanocomposites



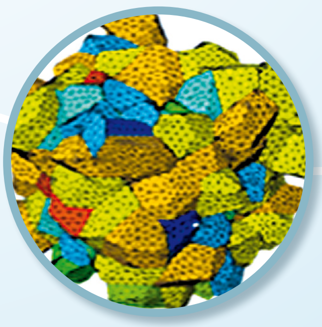
Sustainable Metallurgy

Nanomechanics y Micromechanics

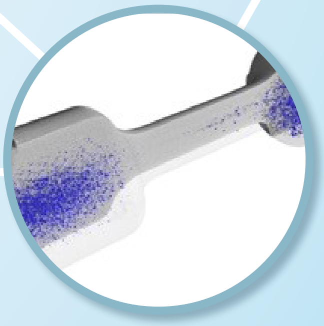
Structural Composites



Bio/Chemo/Mechanics of Materials



Multiscale Materials Modelling



X-Ray Characterisation of Materials

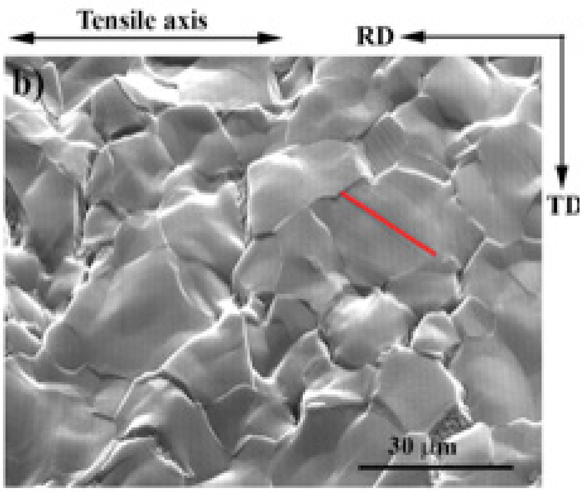
Main research lines

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

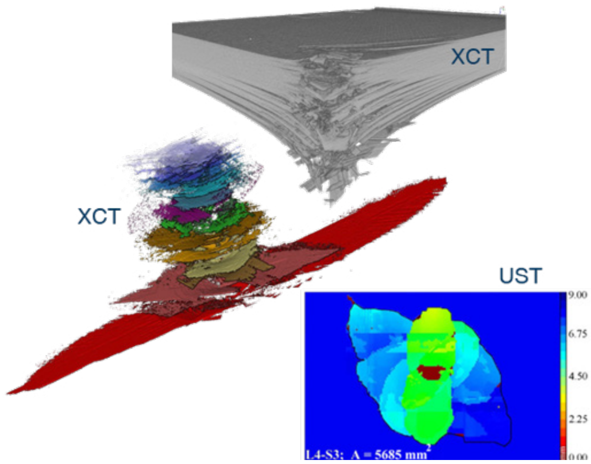
- Multiscale characterisation with optical and electron microscopy, X-rays, atom force microscopy, Raman spectroscopy, ultrasonic inspection. Some of the equipment we use for this are:
  - FIB-FEG-SEM, including 3D-EDS and 3D-EBSD. In-situ stages for thermomechanical testing
  - FEG-TEM including 3D-STEM 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.
- 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.
- Spectroscopic/microscopic studies and implementation in electrochemical energy storage devices such as Li-ion, Na-ion, Li-S and Li-O_2.

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

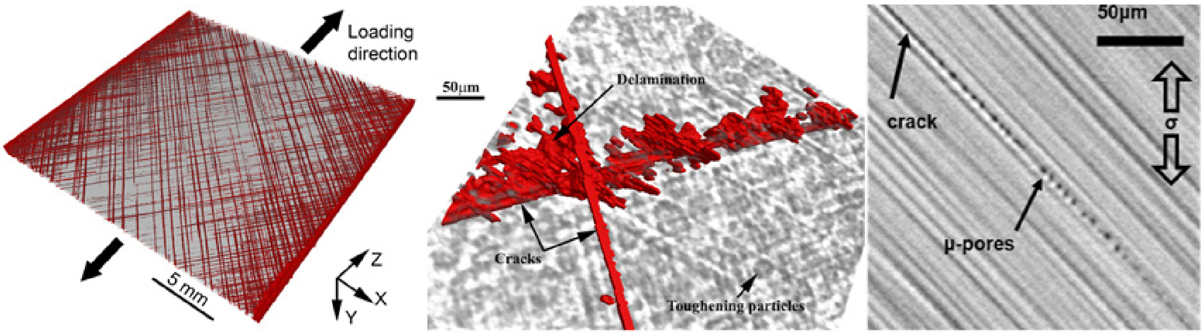


Automatic damage extraction of 3D volumes by XCT and AI correlative techniques

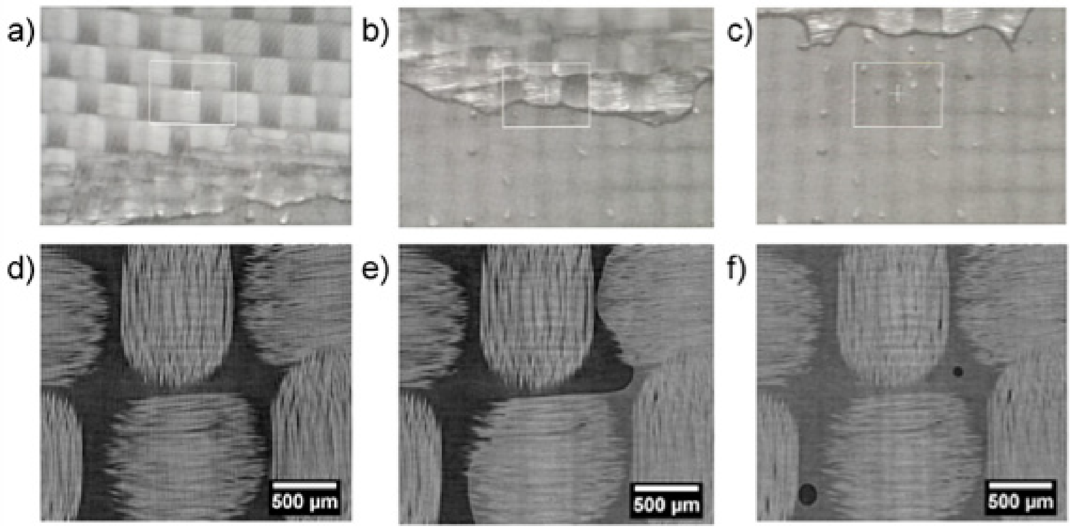
- Properties and deformation mechanisms of small volumes by nanomechanical testing in the scanning and transmission electron microscopes: properties of metallic phases, interfaces, nanoparticles, carbon-based nanomaterials (carbon nanotubes, graphene, etc).
- Elevated temperature nanomechanical testing.
- 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.

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

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

Funding: Regional Government of Madrid/Industrial Doctorate
Partners: Nano4Energy and IMDEA Materials Institute
Project period: 2019 – 2022
Principal Investigators: Dr. J. M. Molina-Aldareguia and Dr. M. Monclús

Figure 1: coated cutting tools

Hard coatings are essential to increase performance in various applications: as wear-resistant coatings for cutting tools and protective coatings for die casting, injection moulding and metal forming. Aluminium titanium nitride ($Al_xTi_{1-x}N$) coatings are currently the most versatile

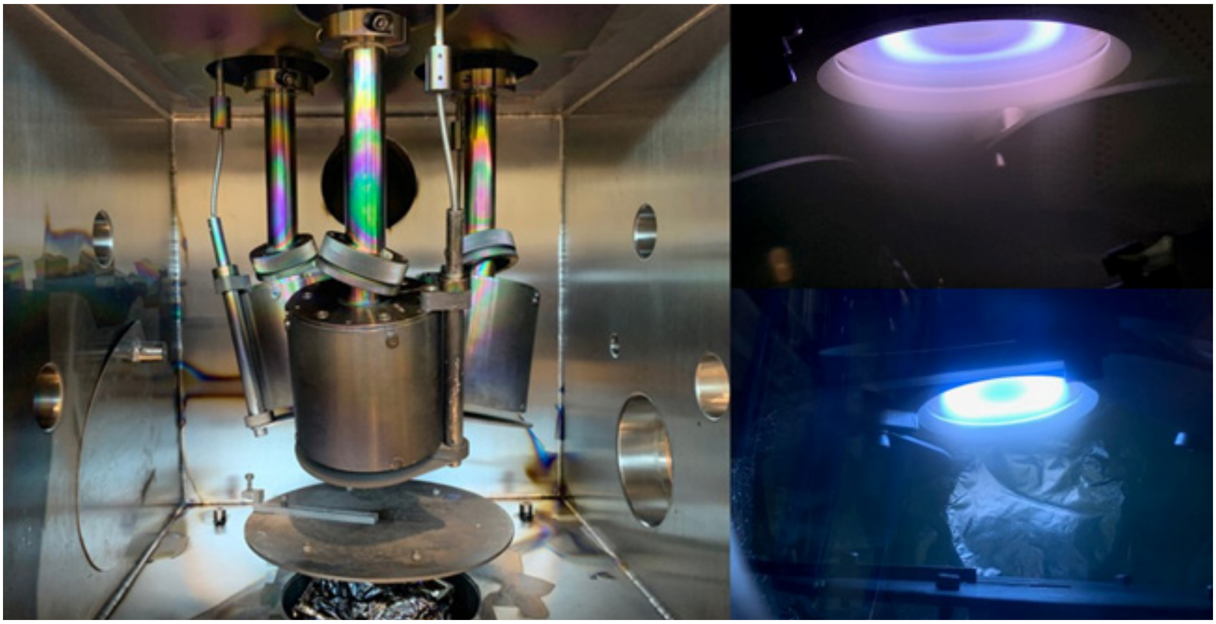


Figure 2. Lab-scale PVD reactor equipped with three magnetrons set up at IMDEA Materials for rapid screening of new coatings

coatings used in industry. They offer a superior wear, oxidation and corrosion resistance over conventional TiN coatings, which contributes to improve the durability of cutting tools (Figure 1). During the last three years, IMDEA Materials Institute and the company Nano4energy have been collaborating through an Industrial Doctorate funded by the Regional Government of Madrid, with the objective of developing new design principles for hard and tough wear resistant coatings.

The most relevant highlights of this project have been:

- A new laboratory-scale Physical Vapour Deposition (PVD) reactor, which includes three magnetrons, has been set up at the Institute that allows for rapid screening of novel compositions and/or processing conditions to develop new coatings (Figure 2).

- Exploration of the benefits of high power impulse magnetron sputtering (HiPIMS), which has the potential to produce much denser coatings at higher deposition rates, thanks to the high energy ion bombardment conditions.

- Development of new AlTiBN coatings with improved high-temperature properties. B doping leads to grain refinement in the coatings, which breaks down the intrinsic columnar microstructure characteristic of AlTiN coatings (Figure 3) and the thermal stability and the hot hardness are substantially enhanced, from 850 ºC to 1000 ºC [1]

[1] A. Mendez, M. A, Monclus, J. A. Santiago, I. Fernandez-Martinez, T. C. Rojas, J. Garcia-Molleja, M. Avella, N. Dams, M. Panizo-Laiz, J. M. Molina-Aldareguia, *Effect of Al content on the hardness and thermal stability study of AlTiN and AlTiBN coatings deposited by HiPIMS*, **Surface and Coatings Technology 422**, 127513 (2021)

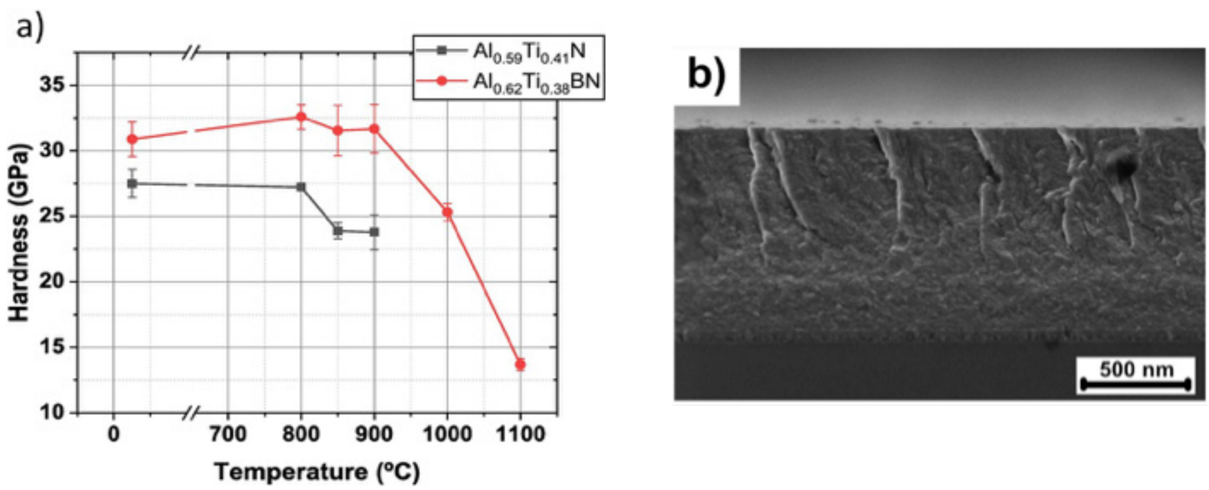


Figure 3. a) Hardness versus temperature of the new AlTiBN coatings, with respect to the AlTiN standard, and b) cross-section of AlTiBN coating that shows the grain refinement effect.

Research highlights

New bioabsorbable and personalized implants through 3D printing

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

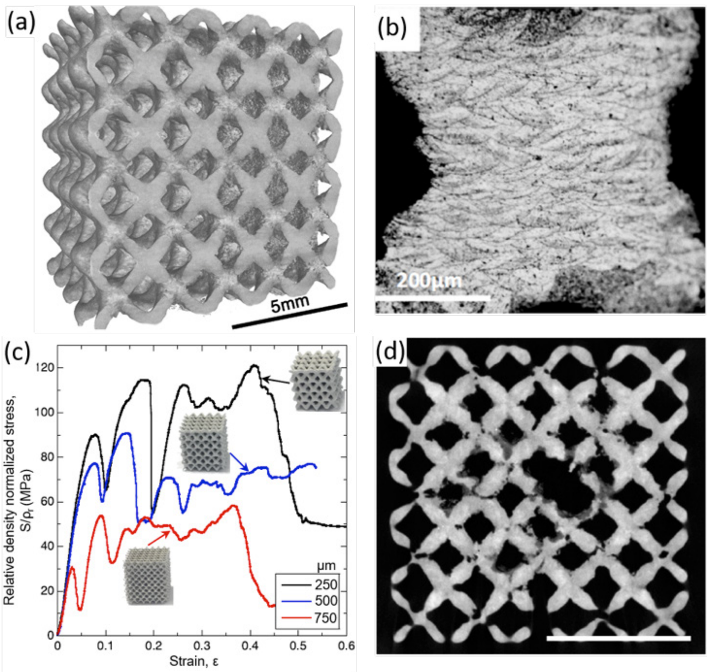


Figure 1. a) Tomography of a WE43 scaffold manufactured by SLM. b) Microstructure of the scaffold. c) Normalized compressive stress curves with the relative density of the scaffold vs strain for different sizes of struts (250 µm, 500 µm and 750 µm). d) Interior of the scaffold after degradation. Adapted from [1].

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, capable of withstanding mechanical loads, having an open porosity that allows vascularization 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 Figure 1a. The microstructure of the material generated by this manufacturing process observed with an optical microscope is shown in Fig. 1b. 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 Figure 1c) 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 (Figure 1d) 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 (Figure 1b) and geometric information will be used to develop numerical models of its mechanical response (Figure 2), with a view to its future integration in models of mechanoregulation of growth and regeneration of bone tissue using porous alloy-based scaffolds.

For more information, please contact:
Dr. Federico Sket at federico.sket@imdea.org

[1] M. Li, F. Benn, T. Derra, N. Kröger, M. Zinser, R. Smeets, J.M. Molina-Aldareguia, A. Kopp, J. Llorca. *Microstructure, mechanical properties, corrosion resistance and cytocompatibility of WE43 Mg alloy scaffolds fabricated by laser powder bed fusion for biomedical applications*, **Material Science and Engineering C 119**, 111623 (2021).

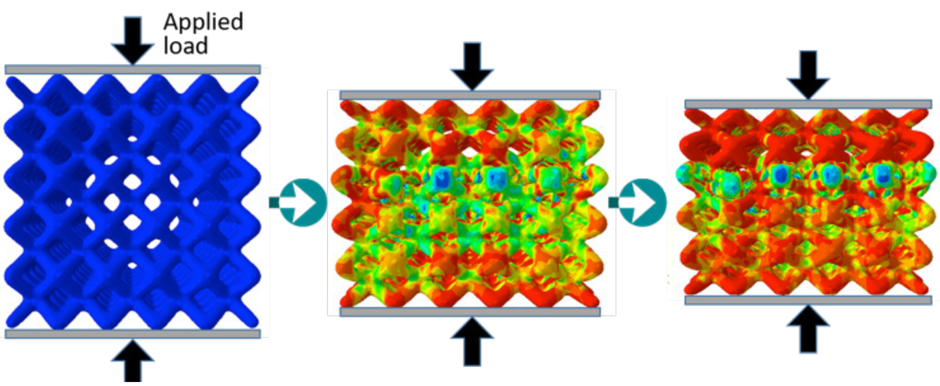


Figure 2. Simulation of the efforts generated in the scaffolding after the application of mechanical loads

Nanoindentation for extreme conditions

Over the past 30 years, nanoindentation testing has become increasingly popular for the mechanical characterization of materials. It is a very versatile technique that allows testing of small volumes or thin films that could not be tested otherwise by macroscale techniques. Furthermore, little test preparation is required and a large amount of data can be obtained in a short time, which is convenient for statistical analysis. One of the main research drivers in the last few years in the area of small scale mechanical testing has been to perform these tests at non-standard conditions, such us at high temperature and/or reactive environments, to allow testing materials as close as possible to their service conditions. One example is the use of this technique to study the high strain rate mechanical behaviour of materials at the micrometer scale. This is motivated by the need to understand how materials deform under high speed events, found for example in machining and forming processes and/or in materials subjected to impacts.

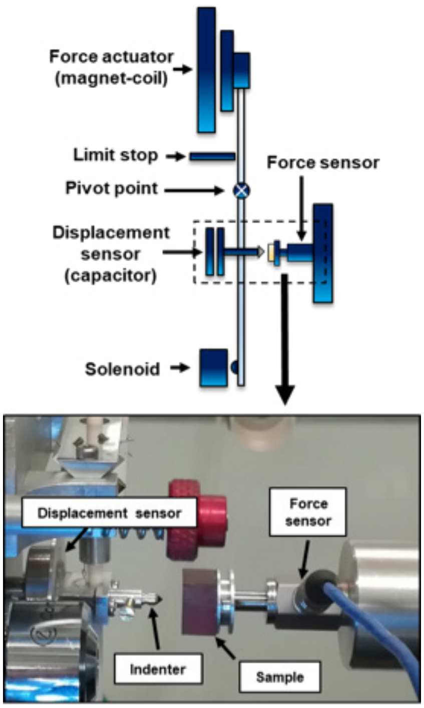


Figure 1.NanoTest pendulum based nanoindenter including the force sensor

In the framework of the European project DYNACOMP, researchers at IMDEA Materials Institute have recently developed strategies to test materials at high strain rates at the microscale [2]. For this, an existing nanoindentation instrument, a Nanotest from Micro Materials Ltd., was instrumented to enable force-displacement measurements in a nano-impact test [3]. Figure 1 shows the schematics of the pendulum-based nanoindenter and the location of the force sensor. The sensor is in direct contact with the sample back surface so that the total applied force in the material surface can be measured. In the NanoTest, force is actuated in the magnet-coil couple, while two capacitor plates in line with the indenter are used for displacement measurement. The pendulum rotates around a frictionless pivot and it uses a limit stop to have a fixed position in space. The nano-impact test is carried out with the assistance of a solenoid located at the base of the instrument. Before impact, the solenoid switches on at the same time than a constant current is applied in the force actuator (the impulse force). The sample surface is positioned at a predefined distance from the indenter (the impulse distance). Then, the solenoid voltage is switched off and the pendulum swings towards the material surface driven by the acceleration given by the impulse force.

The new instrumentation presents several advantages:

- It provides the full load-displacement curve during nano-impact test, which cannot be otherwise determined.
- The ISO-14577 standard for hardness and elastic modulus based on the analysis of the unloading curve can be applied.
- Methods for zero-point correction recommended in the ISO-14577 can be applied.

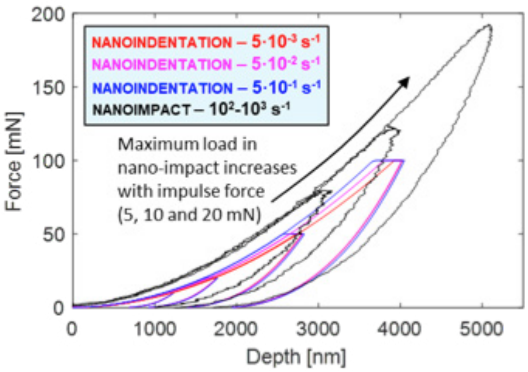


Figure 2. Nanoindentation load-displacement curves obtained at quasi-static and impact conditions in an epoxy resin

- It opens the door to quantitative testing beyond nanoindentation: microcantilever test, micropillar compression, fibre push-in/push-out test, etc.

This new capability was used, for instance, to test the strain rate sensitivity of epoxy resins typically used in aeronautical grade composites. Figure 2 presents the force-displacement curves of the resin during nanoindentation tests performed both at quasi-static conditions (strain rates of 0.005, 0.05 and 0.5 s^{-1}) and under impact conditions (strain rate of 100 s^{-1}). The resin shows a marked strain rate sensitivity, which is materialized in the decreasing depth at constant load with the increase in strain rate.

Moreover, the new instrumentation can also be used to perform other advanced micromechanical tests, such as micropillar compression. Figure 3. shows stress-strain curves at increasing displacement rates, obtained by testing micropillars carved by focused ion beam (FIB) milling in the same epoxy resin. The pillars had a diameter of 7 µm diameter, a size at which the results were found to be representative of the bulk behavior of the material [4]. This new capability opens the door for the quantitative study of the mechanical behavior of materials under impact conditions at the micrometer scale.

For more information, please contact:

Dr. Jon Molina-Aldareguia at jon.molina@imdea.org

[1] https://cordis.europa.eu/project/id/722096

[2] https://www.youtube.com/watch?v=9OgGmHvqWAM

[3] M. Rueda-Ruiz, B. D. Beake, J. M. Molina-Aldareguia, *New instrumentation and analysis methodology for nano-impact testing*, **Materials and Design 192**, 108715 (2020)

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

(a) (b)

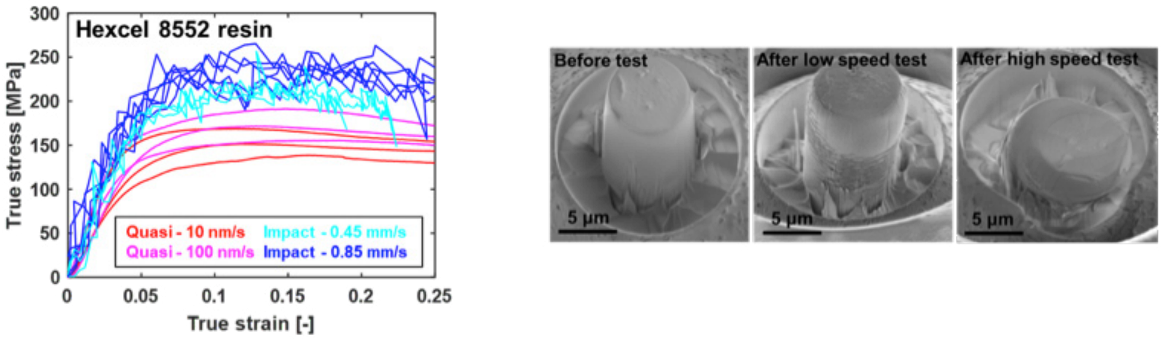


Figure 3. (a) Micropillar stress-strain curves obtained at increasing strain rates and (b) Deformed micropillars.

Materials for Health Care

A new research line on Materials for Health Care became fully operational at the Institute in 2021. In February, Dr. Jennifer Patterson (PhD in Bioengineering from the University of Washington) joined us to lead a new research group on Biomaterials and Regenerative Medicine. She strongly reinforced our research groups already working in the field since 2018. By the end of the year, a fully equipped cell culture and biomaterials laboratory was running (see Figure 1 and the “facilities” section for more details).

This new research facility, co-funded by Madrid Regional Government and by the State Research Agency via the “María de Maeztu” program, allows us to analyse the response of living tissue to new tools, prostheses or devices for medical use that are also being investigated at the Institute (see ongoing projects below). The laboratory consists of a 33 m^2 Biological Safety Level-1 (BSL-1) room and a 29 m^2 BSL-2 area equipped with biosafety cabinets.

The following four research projects are currently running at our Institute in this area:

1. **BioImplant ITN - European Training Network to develop Improved Bioresorbable Materials for Orthopaedic and Vascular Implant Applications** (European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions - ITN - EID)

   Combining polymer-, metal- and ceramic-based bioabsorbable materials, to deliver functionally superior bioabsorbable materials with enhanced mechanical behaviour and controllable degradation profiles.

2. **i-MPLANTS-CM - Metamaterial printing using shape memory alloys and functional gradients for a new generation of smart implants** (Regional Government of Madrid - Synergy projects)

   Printing of metamaterials with shape memory alloys and functional gradients of properties. Development of intelligent implants, which will be implanted through minimally invasive procedures and will be able to evolve geometrically with the patients, shifting their shapes, according to the healing, growth and ageing processes.

3. **MAMAP-CM - Materials and models against pandemic** (Regional Government of Madrid - REACT-EU)

   Materials design and development, device manufacturing, modelling and simulation to protect, fight and forecast pandemic expansion. Including the development of: i) biodegrabdable, biobased micro composites to deactivate viruses, ii) 3D in vitro models of airway tissues and iii) computational model of pandemic spread.

4. **BIOMET4D - Smart 4D biodegradable metallic shape-shifting implants for dynamic tissue restoration** (European Commission/Horizon Europe Programme – EIC pathfinder open)

   Development of shape-shifting and load-bearing implants for dynamic tissue restoration and to introduce a revolutionary paradigm in how actuators can be implemented in biomedicine. Science-towards-technology breakthroughs will be demonstrated with new shape-morphing metamaterials, 4D smart metallic actuators and advanced multi-domain optimization tools.

Figure 1. Cell culture and biomaterials laboratory at IMDEA Materials Institute.

principal investigators

Senior Researchers

Prof. José Manuel Torralba

Director. Sustainable Powder Metallurgy

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

Research Interests

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

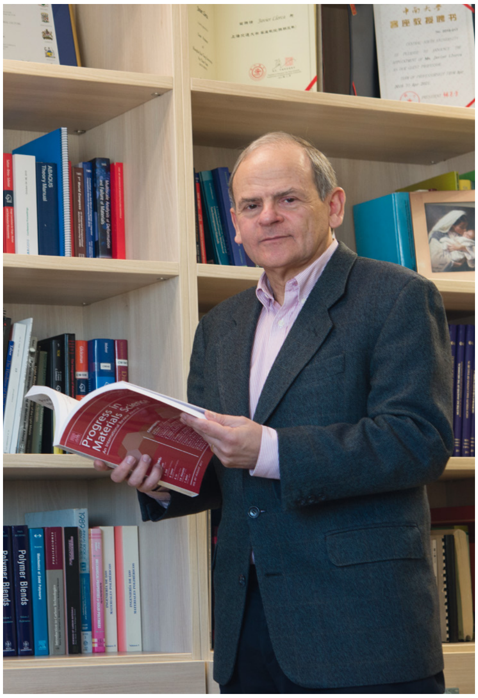
Dr. Jon M. Molina-Aldareguía

Deputy Director. Micromechanics and Nanomechanics

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

Research Interests

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



Prof. Javier LLorca

Scientific Director, Bio/Chemo/Mechanics of Materials

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

Professor of Materials Science, Technical University of Madrid

Research Interests

Development of 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 characterization 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.).

Prof. Carlos González

Senior Researcher,
Structural Composites

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

Professor of Materials Science, Technical University of Madrid

Research Interests

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

Dr. Maciej Haranczyk

Senior Researcher,
Computational and Data-Driven Materials Discovery

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

Research Interests

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

Dr. María Teresa Pérez-Prado

Senior Researcher, Sustainable Metallurgy

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

Research Interests

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

Prof. Ignacio Romero

Senior Researcher, Computational Solid Mechanics

Ph.D. in Civil Engineering, from University of California Berkeley. USA

Professor of Mechanics, Technical University of Madrid

Research Interests

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

Dr. Ilchat Sabirov

Senior Researcher, Physical Simulation

Ph.D. in Metallurgy from Montanuniversitaet Leoben. Austria

Research Interests

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

Dr. Javier Segurado

Senior Researcher, Multiscale Materials Modelling

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

Associate Professor of Materials Science, Technical University of Madrid

Research Interests

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

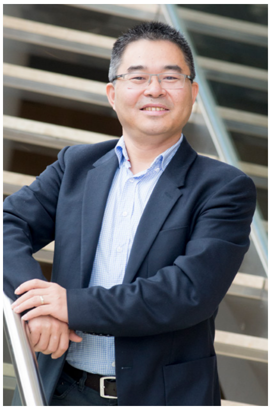
Dr. Srdjan Milenkovic

Senior Researcher,
Solidification Processing & Engineering

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

Research Interests

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



Dr. De-Yi Wang

Senior Researcher,
High Performance Nanocomposites

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

Research Interests

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

Dr. Juan José Vilatela

Senior Researcher,
Multifunctional Nanocomposites

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

Research Interests

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

Researchers

Dr. Vinodkumar Etacheri

Researcher, Electrochemical Energy Storage, Nanomaterials

Ph.D. in Materials Chemistry from Dublin Institute of Technology. Ireland

Research Interests

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

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; characterization 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.

Dr. Federico Sket

Researcher, In-situ processing and mechanical characterization of materials

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

Research Interests

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

Dr. Damien Tourret

Researcher, Modelling and Simulation of Materials Processing

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

Research Interests

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

Visiting Scientists

Dr. 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, California, USA.

Dr. Dan Mordehai
Visiting Researcher

Ph.D. in Physics from the Tel Aviv University, Israel

Associate Professor of Mechanical Engineering at Technion, Haifa, Israel.

Dr. Álvaro Ridruejo
Visiting Researcher

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

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

Ignacio López. Winner of the imaging contest 2022 (characterization)

annex

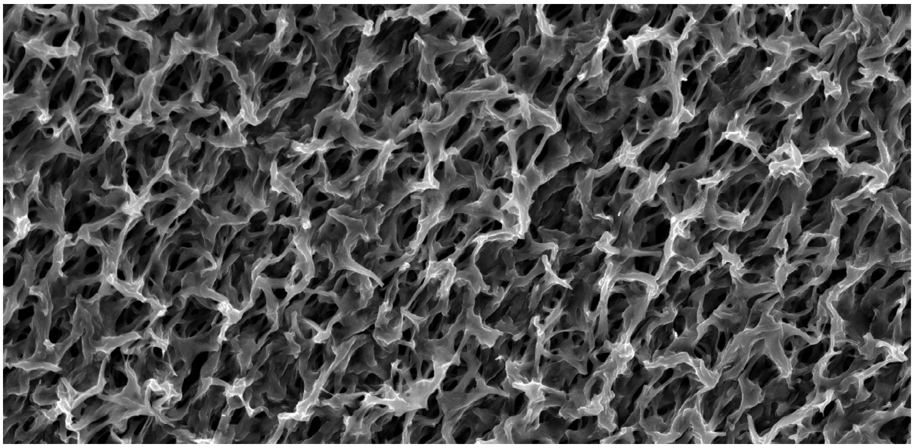
1. R&D projects and contracts

1.1. European R&D Projects (European Commission)

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, 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

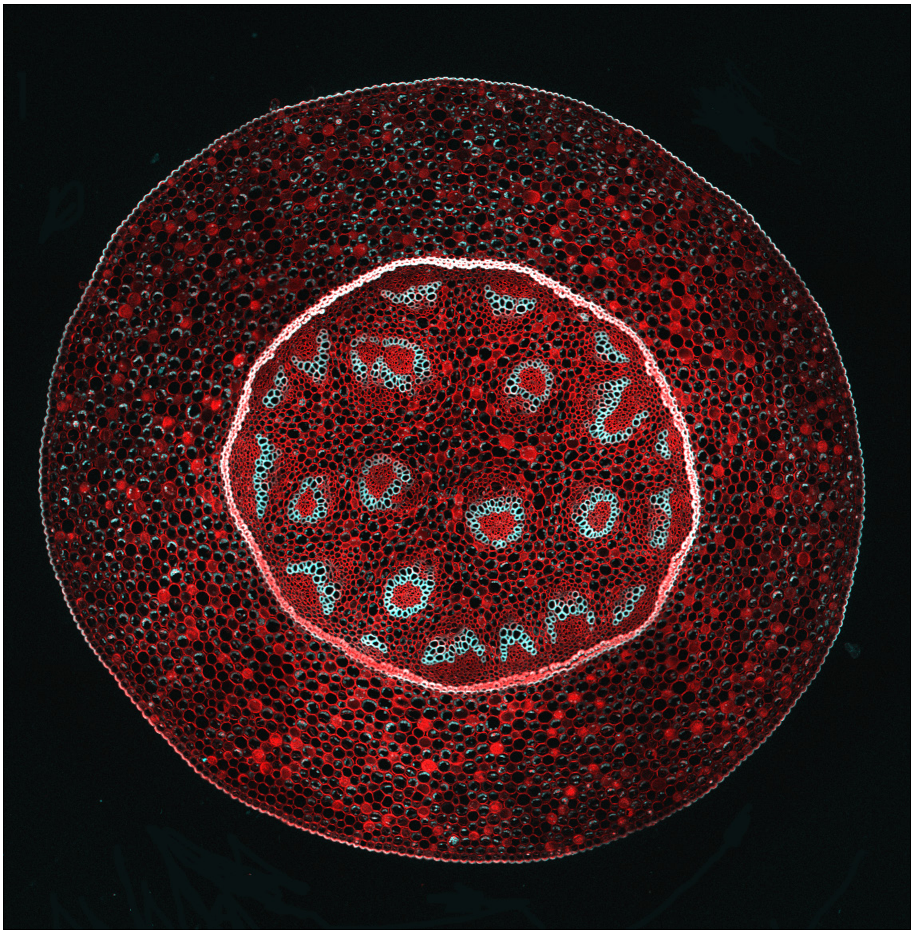
Title/Acronym: Functionally Metalized Nanocellulose For Future Smart Materials/ FUNMAT
Partners: IMDEA Materials Institute
Period: 2020 - 2021
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Marie Skłodowska-Curie actions – IF
Principal Investigator: Dr. A. Azizi; Supervisor: Dr. D-Y Wang



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

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

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

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

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

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

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

Egg drop challenge performed as part of the MOAMMM project. The goal was to design an additive-manufactured metamaterial to effectively prevent an egg from being destroyed from a 2-meter free fall

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

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

Title/Acronym: Structural power composites for future civil aircraft/SORCERER
Partners: Imperial College (Coordinator), Chalmers University of Technology, KTH Royal Institute of Technology, IMDEA Materials Institute
Period: 2017 – 2021
Funding Institution/Programme: European Commission/Horizon 2020 Programme – Clean Sky Joint Undertaking 2
Principal Investigator: Dr. J. J. Vilatela

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

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

1.2. Other International R&D Projects

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

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

1.3. National R&D Projects

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/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigator: Dr. D-Y Wang

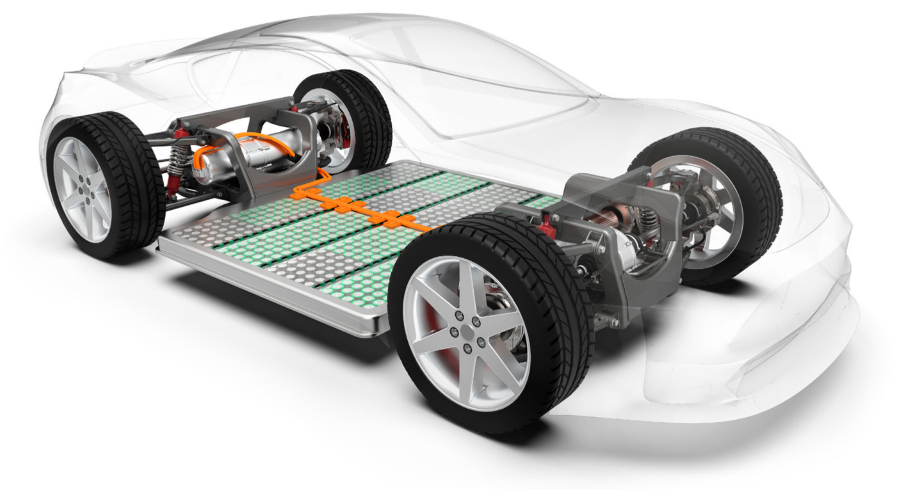
Title/Acronym: X-ray microtomograph with capacity for in situ testing and laboratory based diffraction contrast tomography/LAB-BASED DCT
Partners: IMDEA Materials Institute
Period: 2021 - 2023
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Scientific and Technical Infrastructures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

Title/Acronym: European Project Office IMDEA Materials Institute 2020/(OPE - IMDEA Materials 2020)
Partners: IMDEA Materials Institute
Period: 2021 - 2022
Funding Institution/Programme: Spanish Ministry of Science and Innovation/Europa Networks and Managers - Europa Technology Centres
Coordinator: Miguel Ángel Rodiel

Title/Acronym: Advanced materials and nanomaterials Spanish technological platform/ MATERPLAT
Partners: IMDEA Materials Institute (Technical Secretariat)
Period: 2020 – 2021
Funding Institution/Programme: Spanish Ministry of Science and Innovation/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Technological Platforms
Coordinator: Miguel Ángel Rodiel

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

Title/Acronym: 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/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigators: Dr. J. M. Molina-Aldareguia and Dr. F. Sket



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

Title/Acronym: Spanish network of multiscale materials modelling/ROSALES
Partners: Multiple partners coordinated by CIEMAT (Coordinator)
Period: 2020 - 2021
Funding Institution/Programme: Spanish Ministry of Science and Innovation/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Networks of Excellence
Principal Investigator: Prof. J. LLorca

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

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 Investigators: Dr. J. M. Molina-Aldareguia

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

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

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

UNIT OF EXCELLENCE MARÍA DE MAEZTU

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

Title/Acronym: Virtual environment for the design and manufacturing of airplane turbine engines/ENVIDIA
Partners: ITP Aero (Coordinator), Technical University of Madrid, University of the Basque Country, IMDEA Materials Institute
Period: 2018 – 2021
Funding Institution/Programme: Spanish Ministry of Science and Innovation/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Collaboration Challenges
Principal Investigators: Prof. I. Romero, Prof. J. Segurado and Dr. D. Tourret

Title/Acronym: Quest for safe and sustainable batteries using Na-ion, Mg and hybrid concepts/NAMBAT
Partners: University of Córdoba (Coordinator), IMDEA Materials Institute
Period: 2018 – 2021
Funding Institution/Programme: Spanish Ministry of Science and Innovation/National Programme of Research, Development and Innovation Oriented Challenges of the Society. Research Challenges
Principal Investigators: Dr. V. Etacheri and Dr. M. Haranczyk

Title/Acronym: Ultrafine eutectics by laser additive manufacturing/ELAM
Partners: German Aerospace Research Center (DLR, Coordinator), Access e.V., Wigner Research Centre for Physics, Fraunhofer Institute for Laser Technology, Bosch-Mahle Turbosystems GmbH, P&G Manufacturing GmbH, IMDEA Materials Institute
Period: 2017 – 2021
Funding Institution/Programme: Spanish Ministry of Science and Innovation - European Commission/M-ERA.Net
Principal Investigator: Dr. F. Sket and Dr. S. Milenkovic

1.4. Regional R&D Projects

Title/Acronym: Metamaterial printing using shape memory alloys and functional gradients for a new generation of smart implants/i-MPLANTS-CM
Partners: 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
Doctoral Researcher: Sergi Bafaluy Ojea
Principal Investigator and Supervisor: Dr. M. T. Pérez-Prado

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

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

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

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

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

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

1.5. Privately-funded R&D Projects

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

Title/Acronym: Evaluation of the potential application of earth oxide in flame retardant/REOCABLE
Company: 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

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

Title/Acronym: Study on biobased wood fibre reinforced polymer composites/ BIOCOMPOSITE
Company: University of Strathclyde Glasgow
Period: 2020 - 2021
Principal Investigator Dr. D-Y Wang

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

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

Title/Acronym: Advanced characterization of high-temperature metallic parts fabricated by additive manufacturing/JANO
Company: ITP Aero
Period: 2019 - 2021
Principal Investigators: Dr. M. T. Pérez-Prado and Dr. F. Sket

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

Title/Acronym: Evaluation of damage made by ballast impact in composite materials/ BINOMIAL
Company: Patentes TALGO
Period: 2019-2021
Principal Investigator: Prof. C. González

Title/Acronym: Development of high-performance hydromagnesite-based fillers to polymers/HIGHFILL
Company: Liaoning Jinghua New Materials
Period: 2019-2021
Principal Investigator: Dr. D-Y Wang

Title/Acronym: Eco-friendly Fire Retardant Materials as Fireproof Coating/FIRECOAT
Company: Zhejiang RUICO New Material
Period: 2019-2021
Principal Investigator: Dr. D-Y Wang

Title/Acronym: Development of batteries on flexible plastic substrates/BATFLEX
Company: Grupo Antolin
Scientific Partner: IMDEA Energy
Period: 2018-2021
Principal Investigator: Dr. J. J. Vilatela and Dr. R. Marcilla

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

Title/Acronym: Superalloys for additive manufacturing/SAM
Company: Renishaw Ibérica
Period: 2018-2021
Principal Investigators: Dr. M. T. Pérez-Prado and Prof. J. LLorca

1.6. Licenses

Nanowires network (EP19382996.7)
Type: Patent license
Licensors: IMDEA Materials Institute
Licensee: Floatech, S.L.
Period: 2021 - 2026
Principal Investigator: Dr. J. J Vilatela

Nanowires network (EP21382408.9)
Type: Patent license
Licensors: IMDEA Materials Institute
Licensee: Floatech, S.L.
Period: 2021 - 2026
Principal Investigator: Dr. J. J Vilatela

VIPER - Virtual Ply Property Predictor
Type: Academic purposes royalty-free software license
Licensors: IMDEA Materials Institute
Licensee: International Islamic University Malaysia – Department of Manufacturing and Materials Engineering (Malaysia)
Period: 2021 - 2024
Principal Investigator: Prof. C. González

VIPER - Virtual Ply Property Predictor
Type: Academic purposes royalty-free software license
Licensors: IMDEA Materials Institute
Licensee: Arts et Métiers Metz Campus – Department of Mechanical Engineering (France)
Period: 2021 - 2024
Principal Investigator: Prof. C. González

FFTMAD - Fast Fourier Transform Based Homogenization Code, MADrid
Type: Academic purposes royalty-free software license
Licensors: IMDEA Materials Institute
Licensee: Université de Mostaganem Abdelhamid Ibn Badis (Algeria)
Period: 2021 - 2022
Principal Investigator: Prof. J. Segurado

2. Fellowships

2.1. International

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

Programme: China Scholarship Council fellowships
Project: Multifunctional nanomaterials based polymer nanocomposites
Period: 2016-2021
Funding Institution: China Scholarship Council
J. Zhang

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

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

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

1.2. National

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

Programme: Ramón y Cajal
Period: 2020-2022
Funding Institution: Spanish Ministry of Science and Innovation
Dr. V. Etacheri

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

Programme: Training University Lecturers (FPU)
Period: 2018-2021
Funding Institution: Spanish Ministry of Universities
R. Santos

Programme: Training University Lecturers (FPU)
Period: 2017-2021
Funding Institution: Spanish Ministry of Universities
A. Fernández

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

Programme: Predoctoral Fellowships
Period: 2018-2021
Funding Institution: Spanish Ministry of Science and Innovation
C. Gutierrez

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

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

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

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

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

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

1.3. Regional

Programme: Talent Attraction Programme – Modality 1
Period: 2018-2022
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: 2020-2021
Funding Institution: Madrid Regional Government
A. León

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

Mónica Echeverry. Winner of the imaging contest 2022 (open subject)

3. Scientific results

3.1. Publications

1. Rana M., Boaretto N., Mikhalchan A., Vila Santos M., Marcilla R., Vilatela J.J. *Composite Fabrics of Conformal MoS2Grown on CNT Fibers: Tough Battery Anodes without Metals or Binders*. **ACS APPLIED ENERGY MATERIALS 4**, 5668-5676, 2021.
2. Yuan Y., Pan Y.-T., Zhang W., Feng M., Wang N., Wang D.-Y., Yang R. *Delamination and Engineered Interlayers of Ti3C2MXenes using Phosphorous Vapor toward Flame-Retardant Epoxy Nanocomposites*. **ACS APPLIED MATERIALS AND INTERFACES 13**, 48196-48207, 2021.
3. Feng W., Avvaru V.S., Maça R.R., Hinder S.J., Rodríguez M.C., Etacheri V. *Realization of High Energy Density Sodium-Ion Hybrid Capacitors through Interface Engineering of Pseudocapacitive 3D-CoO-NrGO Hybrid Anodes*. **ACS APPLIED MATERIALS AND INTERFACES 13**, 27999-28009, 2021.
4. Duan Y., Yin G.-Z., Wang D.-Y., Costa R.D. *In Situ Ambient Preparation of Perovskite-Poly(l -lactic acid) Phosphors for Highly Stable and Efficient Hybrid Light-Emitting Diodes*. **ACS APPLIED MATERIALS AND INTERFACES 13**, 21800-21809, 2021.
5. Unnikrishnan V., Zabihi O., Li Q., Ahmadi M., Yadav R., Kalali E.N., Tanwar K., Kiziltas A., Blanchard P., Wang D.-Y., Naebe M. *Organophosphorus-Functionalized Zirconium-Based Metal–Organic Framework Nanostructures for Improved Mechanical and Flame Retardant Polymer Nanocomposites*. **ACS APPLIED NANO MATERIALS 4**, 13027-13040, 2021.
6. Vila M., Hong S., Park S., Mikhalchan A., Ku B.-C., Hwang J.Y., Vilatela J.J. *Identification of Collapsed Carbon Nanotubes in High-Strength Fibers Spun from Compositionally Polydisperse Aerogels*. **ACS APPLIED NANO MATERIALS 4**, 6947-6955, 2021.
7. Zabihi O., Ahmadi M., Yadav R., Mahmoodi R., Naderi Kalali E., Nikafshar S., Ghandehari Ferdowsi M.R., Wang D.-Y., Naebe M. *Novel Phosphorous-Based Deep Eutectic Solvents for the Production of Recyclable Macadamia Nutshell-Polymer Biocomposites with Improved Mechanical and Fire Safety Performances*. **ACS SUSTAINABLE CHEMISTRY AND ENGINEERING 9**, 4463-4476, 2021.
8. Shi D.F., Wang C.Y., Cepeda-Jiménez C.M., Pérez-Prado M.T. *Atomic scale interactions of basal dislocations and twin boundaries with ultrathin precipitates in magnesium alloys*. **ACTA MATERIALIA 221**, 2021.
9. Li N., Wang C., Monclús M.A., Yang L., Molina-Aldareguia J. M. *Solid solution and precipitation strengthening effects in basal slip, extension twinning and pyramidal slip in Mg-Zn alloys*. **ACTA MATERIALIA 221**, 2021.
10. Wang J., Chen Y., Chen Z., LLorca J., Zeng X. *Deformation mechanisms of Mg-Ca-Zn alloys studied by means of micropillar compression tests*. **ACTA MATERIALIA 217**, 2021.

11. Bellón B., Boukellal A.K., Isensee T., Wellborn O.M., Trumble K.P., Krane M.J.M., Titus M.S., Tourret D., LLorca J. *Multiscale prediction of microstructure length scales in metallic alloy casting*. **ACTA MATERIALIA 207**, 2021.
12. Valencia F.J., Santiago J., González R.I., González-Arrabal R., Ruestes C., Perez Díaz M., Monclus M.A., Molina-Aldareguia J. M., Nuñez P.D., Munoz F., Kiwi M., Perlado J.M., Bringa E.M. *Nanoindentation of Amorphous Carbon: a combined experimental and simulation approach*. **ACTA MATERIALIA 203**, 2021.
13. Gebhardt C.G., Romero I. *On a nonlinear rod exhibiting only axial and bending deformations: mathematical modeling and numerical implementation*. **ACTA MECHANICA 232**, 3825-3847, 2021.
14. Galera-Rueda C., Montero-Sistiaga M.L., Vanmeensel K., Godino-Martínez M., LLorca J., Pérez-Prado M.T. *Icosahedral quasicrystal-enhanced nucleation in Al alloys fabricated by selective laser melting*. **ADDITIVE MANUFACTURING 44**, 2021.
15. Jacobo-Martín A., Hernández J.J., Pedraz P., Navarro-Baena I., Monclús M.A., Molina-Aldareguia J. M., Rodríguez I. *Enhanced Mechanical and Thermal Resistances of Nanoimprinted Antireflective Moth-Eye Surfaces Based on Poly Vinylidene Fluoride/TiO2 Surface Nanocomposites*. **ADVANCED ENGINEERING MATERIALS 23**, 2021.
16. Duan Y., Wang D.-Y., Costa R.D. *Recent Progress on Synthesis, Characterization, and Applications of Metal Halide Perovskites@Metal Oxide*. **ADVANCED FUNCTIONAL MATERIALS 31**, 2021.
17. 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** (early view), 2021.
18. Karjule N., Rana M., Shalom M., Barrio J., Vilatela J.J. *Controlled Nucleation and Growth of Carbon Nitride Films on CNT Fiber Fabric for Photoelectrochemical Applications*. **ADVANCED SUSTAINABLE SYSTEMS 5**, 2021.
19. Shi Z., Shao W., Rao L., Hu T., Xing X., Zhou Y., Liu S., Yang Q. *Effects of Y dopant on mechanical properties and electronic structures of M7C3 carbide in Fe-Cr-C hardfacing coating*. **APPLIED SURFACE SCIENCE 538**, 2021.
20. Zhou M., Liu Y., Yao D., Jiang Y., Zhang X., Wang D.-Y., Wang N. *Promotion of the flame retardancy of 9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide grafted natural rubber using expandable graphite*. **ARABIAN JOURNAL OF CHEMISTRY 14**, 2021.
21. Maça R.R., Etacheri V. *Effect of vinylene carbonate electrolyte additive on the surface chemistry and pseudocapacitive sodium-ion storage of tio2 nanosheet anodes*. **BATTERIES 7**, 1-21, 2021.
22. Doñoro Á., Muñoz-Mauricio Á., Etacheri V. *High-performance lithium sulfur batteries based on multidimensional Graphene-CNT-Nanosulfur hybrid cathodes*. **BATTERIES 7**, 2021.
23. Piluso S., Skvortsov G.A., Altunbek M., Afghah F., Khani N., Koc B., Patterson J. *3D bioprinting of molecularly engineered PEG-based hydrogels utilizing gelatin fragments*. **BIOFABRICATION 13**, 2021.

24. Mikhalchan A., Vila M., Arévalo L., Vilatela J.J. Simultaneous improvements in conversion and properties of molecularly controlled CNT fibres. CARBON 179, 417-424, 2021.
25. Santos C., Rodríguez I.V., Lado J.J., Vila M., García-Quismondo E., Anderson M.A., Palma J., Vilatela J.J. *Low-energy consumption, free-form capacitive deionization through nanostructured networks*. **CARBON 176**, 390-399, 2021.
26. Madrona C., Vila M., Oropeza F.E., de la Peña O'Shea V.A., Vilatela J.J. *Macroscopic yarns of FeCl3-intercalated collapsed carbon nanotubes with high doping and stability*. **CARBON 173**, 311-321, 2021.
27. Avvaru V.S., Fernandez I.J., Feng W., Hinder S.J., Rodríguez M.C., Etacheri V. *Extremely pseudocapacitive interface engineered CoO@3D-NRGO hybrid anodes for high energy/ power density and ultralong life lithium-ion batteries*. **CARBON 171**, 869-881, 2021.
28. Sun C.-C., Yusuf A., Li S.-W., Qi X.-L., Ma Y., Wang D.-Y. *Metal-organic frameworks enabled rational design of multifunctional PEO-based solid polymer electrolytes*. **CHEMICAL ENGINEERING JOURNAL 414**, 2021.
29. Lo Dico G., Nuñez Á.P., Carcelén V., Haranczyk M. *Machine-learning-accelerated multimodal characterization and multiobjective design optimization of natural porous materials*. **CHEMICAL SCIENCE 12**, 9309-9317, 2021.
30. Shao Z.-B., Cui J., Li X.-L., Díaz Palencia J.L., Wang D.-Y. *Chemically inorganic modified ammonium polyphosphate as eco-friendly flame retardant and its high fire safety for epoxy resin*. **COMPOSITES COMMUNICATIONS 28**, 2021.
31. Yin G.-Z., Díaz Palencia J.L., Wang D.-Y. *Fully bio-based Poly (Glycerol-Itaconic acid) as supporter for PEG based form stable phase change materials*. **COMPOSITES COMMUNICATIONS 27, 2021**.
32. Li X., Zhang J., Zhang L., Ruiz de Luzuriaga A., Rekondo A., Wang D.-Y. *Recyclable flame-retardant epoxy composites based on disulfide bonds: Flammability and recyclability*. **COMPOSITES COMMUNICATIONS 25**, 2021.
33. Zhang J., Li Z., Yin G.-Z., Wang D.-Y. *Construction of a novel three-in-one biomass based intumescent fire retardant through phosphorus functionalized metal-organic framework and β-cyclodextrin hybrids in achieving fire safe epoxy*. **COMPOSITES COMMUNICATIONS 23**, 2021.
34. Shao Z.-B., Zhang J., Jian R.-K., Sun C.-C., Li X.-L., Wang D.-Y. *A strategy to construct multifunctional ammonium polyphosphate for epoxy resin with simultaneously high fire safety and mechanical properties*. **COMPOSITES PART A: APPLIED SCIENCE AND MANUFACTURING 149**, 2021.
35. Fernández A., Santangelo-Muro M., Fernández-Blázquez J.P., Lopes C.S., Molina-Aldareguia J. M. *Processing and properties of long recycled-carbon-fibre reinforced polypropylene*. **COMPOSITES PART B: ENGINEERING 211**, 2021.
36. Pascual-González C., San Martín P., Lizarralde I., Fernández A., León A., Lopes C.S., Fernández-Blázquez J.P. *Post-processing effects on microstructure, interlaminar and thermal properties of 3D printed continuous carbon fibre composites*. **COMPOSITES PART B: ENGINEERING 210**, 2021.

37. Castro J., Sket F., Helfen L., González C. *In situ local imaging and analysis of impregnation during liquid moulding of composite materials using synchrotron radiation computed laminography*. **COMPOSITES SCIENCE AND TECHNOLOGY 215**, 2021.
38. Yu Q., Martínez E., Segurado J., Marian J. *A stochastic solver based on the residence time algorithm for crystal plasticity models*. **COMPUTATIONAL MECHANICS 68**, 1369-1384, 2021.
39. Segurado J., Lebensohn R.A. *An FFT-based approach for Bloch wave analysis: application to polycrystals*. **COMPUTATIONAL MECHANICS 68**, 981-1001, 2021.
40. Schiebl M., Romero I. *Energy-momentum conserving integration schemes for molecular dynamics*. **COMPUTATIONAL MECHANICS 67**, 915-935, 2021.
41. Magri M., Lucarini S., Lemoine G., Adam L., Segurado J. *An FFT framework for simulating non-local ductile failure in heterogeneous materials*. **COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING 380**, 2021.
42. Andreev K., Yin Y., Luchini B., Sabirov I. *Failure of refractory masonry material under monotonic and cyclic loading – Crack propagation analysis*. **CONSTRUCTION AND BUILDING MATERIALS 299**, 2021.
43. Nguyen K., Zhang M., Amores V.J., Sanz M.A., Montáns F.J. *Computational modeling of dislocation slip mechanisms in crystal plasticity: A short review*. **CRYSTALS 11**, 1-29, 2021.
44. del Barrio M., Rana M., Vilatela J.J., Lorenzo E., De Lacey A.L., Pita M. *Photoelectrocatalytic detection of NADH on n-type silicon semiconductors facilitated by carbon nanotube fibers*. **ELECTROCHIMICA ACTA 377**, 2021.
45. Yin G.-Z., Hobson J., Duan Y., Wang D.-Y. *Polyrotaxane: New generation of sustainable, ultra-flexible, form-stable and smart phase change materials*. **ENERGY STORAGE MATERIALS 40**, 347-357, 2021.
46. Tapia-Fernández S., Alonso-Miyazaki P.H., Romero I., García-Beltrán A. *Strategy and algorithms for the parallel solution of the nearest neighborhood problem in shared-memory processors*. **ENGINEERING WITH COMPUTERS** , 2021.
47. Zhang L., Ou Y., Wang D.-Y. *Surface functionalization of carbon fabric towards high-performance epoxy composites via enhanced fiber-matrix interfacial strength and intergrowth charring behavior*. **EXPRESS POLYMER LETTERS 15**, 503-514, 2021.
48. Ruiz-Hitzky E., Ruiz-García C., Fernandes F.M., Lo Dico G., Lisuzzo L., Prevot V., Darder M., Aranda P. *Sepiolite-Hydrogels: Synthesis by Ultrasound Irradiation and Their Use for the Preparation of Functional Clay-Based Nanoarchitectured Materials*. **FRONTIERS IN CHEMISTRY 9**, 2021.
49. Dieringa H., StJohn D., Pérez Prado M.T., Kainer K.U. *Editorial: Latest Developments in the Field of Magnesium Alloys and Their Applications*. **FRONTIERS IN MATERIALS 8**, 2021.
50. Denzer B.R., Kulchar R.J., Huang R.B., Patterson J. *Advanced methods for the characterization of supramolecular hydrogels*. **GELS 7**, 2021.
51. Ruiz D., Portillo D., Romero I. *A data-driven method for dissipative thermomechanics*. **IFAC-PAPERSONLINE 54**, 315-320, 2021.

52. Kulchar R.J., Denzer B.R., Chavre B.M., Takegami M., Patterson J. *A review of the use of microparticles for cartilage tissue engineering*. **INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES 22**, 2021.
53. Marvi-Mashhadi M., Vaz-Romero A., Sket F., Rodríguez-Martínez J.A. *Finite element analysis to determine the role of porosity in dynamic localization and fragmentation: Application to porous microstructures obtained from additively manufactured materials*. **INTERNATIONAL JOURNAL OF PLASTICITY 143**, 2021.
54. Zhang M., Zhang H., Ma A., LLorca J. *Experimental and numerical analysis of cyclic deformation and fatigue behavior of a Mg-RE alloy*. **INTERNATIONAL JOURNAL OF PLASTICITY 139**, 2021.
55. Zhang M., Nguyen K., Segurado J., Montáns F.J. *A multiplicative finite strain crystal plasticity formulation based on additive elastic corrector rates: Theory and numerical implementation*. **INTERNATIONAL JOURNAL OF PLASTICITY 137**, 2021.
56. Cantón-Sánchez R., Romero I. *Dimensionally reduced nonlinear solids with general loads and constitutive laws: Theory and finite element formulation for rod-like bodies*. **INTERNATIONAL JOURNAL OF SOLIDS AND STRUCTURES 210-211**, 273-288, 2021.
57. Becker C.G., Tourret D., Smith D., Rodgers B., Imhoff S., Gibbs J., Hunter J., Espy M., Clarke K., Clarke A. I*ntegrating In Situ x-Ray Imaging, Energy Dispersive Spectroscopy, and Calculated Phase Diagram Analysis of Solute Segregation During Solidification of an Al-Ag Alloy*. **JOM 73**, 3291-3300, 2021.
58. Chen N., Kou H., Wu Z., Qiang F., Wang C., Li J., Molina-Aldareguia J. M. *Stress-induced β' martensitic phase transformation and martensitic twinning in a metastable β titanium alloy*. **JOURNAL OF ALLOYS AND COMPOUNDS 859**, 2021.
59. Tsipas S.A., Tabares E., Weissgaerber T., Hutsch T., Sket F., Velasco B. *Thermophysical properties of porous Ti2AlC and Ti3SiC2 produced by powder metallurgy*. **JOURNAL OF ALLOYS AND COMPOUNDS 857**, 2021.
60. Boehlert C.J., Sabirov I., Ruiz-Palenzuela B., Cornide J., Ruiz-Navas E.M. *A comparison of field assisted hot pressing and hot isostatic pressing for gas atomized Ti–22Al–26Nb(at.%) and Ti–22Al–26Nb–5B(at.%) powders*. **JOURNAL OF ALLOYS AND COMPOUNDS 852**, 2021.
61. Shi Z., Shao W., Rao L., Hu T., Xing X., Zhou Y., Liu S., Yang Q. *Effects of Ce doping on mechanical properties of M7C3 carbides in hypereutectic Fe–Cr–C hardfacing alloy*. **JOURNAL OF ALLOYS AND COMPOUNDS 850**, 2021.
62. Li Z., Bucior B.J., Chen H., Haranczyk M., Siepmann J.I., Snurr R.Q. *Machine learning using host/guest energy histograms to predict adsorption in metal-organic frameworks: Application to short alkanes and Xe/Kr mixtures*. **JOURNAL OF CHEMICAL PHYSICS 155**, 2021.
63. Kancharlapalli S., Gopalan A., Haranczyk M., Snurr R.Q. *Fast and Accurate Machine Learning Strategy for Calculating Partial Atomic Charges in Metal-Organic Frameworks*. **JOURNAL OF CHEMICAL THEORY AND COMPUTATION 17**, 3052-3064, 2021.

Mohammad Elahi. Winner of the imaging contest 2022 (people award)

64. Jin X.Z., Xu W.C., Shan D.B., Guo B., Jin B., Pérez-Prado M.T. *A quantitative microplasticity-based approach to rationalize the poor strengthening response of polycrystalline Mg alloys*. **JOURNAL OF MAGNESIUM AND ALLOYS** , 2021.
65. Orozco-Caballero A., Gutierrez C., Gan B., Molina-Aldareguia J. M. *High-throughput nanoindentation mapping of cast IN718 nickel-based superalloys: influence of the Nb concentration*. **JOURNAL OF MATERIALS RESEARCH 36**, 2213-2222, 2021.
66. Acuña P., Zhang J., Yin G.-Z., Liu X.-Q., Wang D.-Y. *Bio-based rigid polyurethane foam from castor oil with excellent flame retardancy and high insulation capacity via cooperation with carbon-based materials*. **JOURNAL OF MATERIALS SCIENCE 56**, 2684-2701, 2021.
67. Hernández T., Moroño A., Sánchez F.J., Maffiotte C., Monclús M.A., González-Arrabal R. *Study of deuterium permeation, retention, and desorption in SiC coatings submitted to relevant conditions for breeder blanket applications: thermal cycling effect under electron irradiation and oxygen exposure*. **JOURNAL OF NUCLEAR MATERIALS 557**, 2021.
68. Ciurduc D.E., Boaretto N., Fernández-Blázquez J.P., Marcilla R. *Development of high performing polymer electrolytes based on superconcentrated solutions*. **JOURNAL OF POWER SOURCES 506**, 2021.
69. Vincent M., Avvaru V.S., Rodríguez M.C., Haranczyk M., Etacheri V. *High-rate and ultralong-life Mg–Li hybrid batteries based on highly pseudocapacitive dual-phase TiO2 nanosheet cathodes*. **JOURNAL OF POWER SOURCES 506**, 2021.
70. Abando N., Saad H., Monclús M.A., Deville S., Molina-Aldareguia J. M., Roa J.J. *Anisotropy effect of bioinspired ceramic/ceramic composites: Can the platelet orientation enhance the mechanical properties at micro- and submicrometric length scale?*. **JOURNAL OF THE EUROPEAN CERAMIC SOCIETY 41**, 2753-2762, 2021.
71. Ali W., Echeverry-Rendón M., Kopp A., González C., LLorca J. *Strength, corrosion resistance and cellular response of interfaces in bioresorbable poly-lactic acid/Mg fiber composites for orthopedic applications*. **JOURNAL OF THE MECHANICAL BEHAVIOR OF BIOMEDICAL MATERIALS 123**, 2021.
72. Santos-Güemes R., Capolungo L., Segurado J., LLorca J. *Dislocation dynamics prediction of the strength of Al–Cu alloys containing shearable* β''' *precipitates*. **JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS 151**, 2021.
73. Yang Y., Haurie L., Wang D.-Y. *Bio-based materials for fire-retardant application in construction products: a review*. **JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY** , 2021.
74. Guo Y., Zhou M., Yin G.-Z., Kalali E., Wang N., Wang D.-Y. *Basalt fiber-based flame retardant epoxy composites: Preparation, thermal properties, and flame retardancy*. **MATERIALS 14**, 1-15, 2021.
75. Molina-Aldareguia J. M., Sebastiani M., Korsunsky A.M. *Preface – Virtual Special Issue on nanomechanical testing in materials research and development*. **MATERIALS AND DESIGN 199**, 2021.

76. Wang J., Xu G., Zeng X., LLorca J., Cui Y. *Exploring the correlation between solvent diffusion and creep resistance of Mg-Ga HCP alloys from high throughput liquid-solid diffusion couple*. **MATERIALS AND DESIGN 197**, 2021.
77. Boehlert C.J., Hernández-Escobar D., Ruiz-Palenzuela B., Sabirov I., Cornide J., Ruiz-Navas E.M. *The effect of microstructure and strain rate on the 25 °C and 700 °C compression deformation behavior of powder metallurgy processed Ti-45Al-2Nb-2Mn (at.%)-0.8 TiB2 (vol%) alloy*. **MATERIALS CHARACTERIZATION 172**, 2021.
78. Lapcinska S., Revilla-Cuesta A., Abajo-Cuadrado I., Cuevas J.V., Avella M., Arsenyan P., Torroba T. *Dye-modified silica-anatase nanoparticles for the ultrasensitive fluorogenic detection of the improvised explosive TATP in an air microfluidic device*. **MATERIALS CHEMISTRY FRONTIERS 5**, 8097-8107, 2021.
79. Torralba J.M., Venkatesh Kumarán S. *Development of competitive high-entropy alloys using commodity powders*. **MATERIALS LETTERS 301**, 2021.
80. Chao Q., Sabirov I., Guo T., Hodgson P.D., Beladi H. *Tailoring the deformation characteristics of commercial purity titanium through hot deformation of a martensitic microstructure*. **MATERIALS SCIENCE AND ENGINEERING A 827**, 2021.
81. Jin X., Xu W., Yang G., Shan D., Guo B. *Microstructure evolution and strengthening mechanisms of Mg-6Gd-4Y-0.5Zn-0.5Zr alloy during hot spinning and aging treatment*. **MATERIALS SCIENCE AND ENGINEERING A 827**, 2021.
82. Chen N., Kou H., Wu Z., Qiang F., Hua K., Fan J., Tang B., Li J. M., Molina-Aldareguia J.M. *Microstructural sensitivity and deformation micro-mechanisms of a bimodal metastable* β *titanium Ti–7Mo–3Nb–3Cr–3Al alloy*. **MATERIALS SCIENCE AND ENGINEERING A 824**, 2021.
83. Martin A., San Sebastian M., Gil E., Wang C.Y., Milenkovic S., Pérez-Prado M.T., Cepeda-Jiménez C.M. *Effect of the heat treatment on the microstructure and hardness evolution of a AlSi10MgCu alloy designed for laser powder bed fusion*. **MATERIALS SCIENCE AND ENGINEERING A 819**, 2021.
84. Li N., Yang L., Wang C., Monclús M.A., Shi D., Molina-Aldareguía J. M. *Deformation mechanisms of basal slip, twinning and non-basal slips in Mg–Y alloy by micropillar compression*. **MATERIALS SCIENCE AND ENGINEERING A 819**, 2021.
85. Galera-Rueda C., Nieto-Valeiras E., Gardon M., Pérez-Prado M.T., LLorca J. *Effect of ZrH2 particles on the microstructure and mechanical properties of IN718 manufactured by selective laser melting*. **MATERIALS SCIENCE AND ENGINEERING A 813**, 2021.
86. Liu Z., Yuan X., Wang S., Liu S., Tan H.H., Jagadish C. *Nanomechanical behavior of single taper-free GaAs nanowires unravelled by in-situ TEM mechanical testing and molecular dynamics simulation*. **MATERIALS SCIENCE AND ENGINEERING A 806**, 2021.
87. Alizadeh R., Wang J., LLorca J. *Precipitate strengthening of pyramidal slip in Mg–Zn alloys*. **MATERIALS SCIENCE AND ENGINEERING A 804**, 2021.
88. de Oliveira P.C., Montoro L.A., Perez-Prado M.T., Hohenwarter A., Figueiredo R.B., Isaac A. *Development of segregations in a Mg–Mn–Nd alloy during HPT processing*. **MATERIALS SCIENCE AND ENGINEERING A 802**, 2021.

89. Liu Z., Snel J., Boll T., Wang J.Y., Monclús M.A., Molina-Aldareguía J. M., LLorca J. *High temperature strength retention of Cu/Nb nanolaminates through dynamic strain ageing*. **MATERIALS SCIENCE AND ENGINEERING A 799**, 2021.

90. Li M., Benn F., Derra T., Kröger N., Zinser M., Smeets R., Molina-Aldareguia J. M., Kopp A., LLorca J. *Microstructure, mechanical properties, corrosion resistance and cytocompatibility of WE43 Mg alloy scaffolds fabricated by laser powder bed fusion for biomedical applications*. **MATERIALS SCIENCE AND ENGINEERING C 119**, 2021.

91. Liu S., Esteban-Manzanares G., LLorca J. *First Principles Prediction of the Al-Li Phase Diagram*. **METALLURGICAL AND MATERIALS TRANSACTIONS A: PHYSICAL METALLURGY AND MATERIALS SCIENCE 52**, 4675-4690, 2021.

92. García-Junceda A., Rodríguez D., Hernández R., Serrano M. *Investigation of the Effect of 475 °C Aging Treatment on Mechanical Properties of a Fe–19Cr–5.5Al ODS Alloy Using Tensile, Impact and Small Punch Tests*. **METALLURGICAL AND MATERIALS TRANSACTIONS A: PHYSICAL METALLURGY AND MATERIALS SCIENCE 52**, 4500-4509, 2021.

93. Li G., Jadhav S.D., Martín A., Montero-Sistiaga M.L., Soete J., Sebastian M.S., Cepeda-Jiménez C.M., Vanmeensel K. I*nvestigation of Solidification and Precipitation Behavior of Si-Modified 7075 Aluminum Alloy Fabricated by Laser-Based Powder Bed Fusion*. **METALLURGICAL AND MATERIALS TRANSACTIONS A: PHYSICAL METALLURGY AND MATERIALS SCIENCE 52**, 194-210, 2021.

94. Toda-Caraballo I., Jiménez J.A., Milenkovic S., Jimenez-Aguirre J., San-Martín D. *Microstructural stability of the cocrfe2ni2 high entropy alloys with additions of cu and mo*. **METALS 11**, 2021.

95. Torralba J.M. *Powder metallurgy: A new open section in metals*. **METALS 11**, 2021.

96. Garbiec D., Leshchynsky V., García-Junceda A., Swadβba R., Siwak P., Adamek G., Radwaβski K. *Microstructure and mechanical properties of spark plasma sintered and severely deformed aa7075 alloy*. **METALS 11**, 2021.

97. Sabirov I., Santofimia M.J., Petrov R.H. *Advanced high-strength steels by quenching and partitioning*. METALS 11, 2021.

98. Alvaredo-Olmos P., Molina-Aldareguía J. M., Vaz-Romero A., Prieto E., González-Julián J., Monclús M.A. *Understanding the links between the composition-processing-properties in new formulations of heas sintered by sps*. METALS 11, 2021.

99. Campos M., Torralba J.M., de Oro R., Bernardo E., Galánβalazar A. *New opportunities for low alloy steels—master alloys for liquid phase sintering*. **METALS 11**, 1-21, 2021.

100. Cruzado A., Segurado J., Hartl D.J., Benzerga A.A. *A variational fast Fourier transform method for phase-transforming materials*. **MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING 29**, 2021.

101. Yang Y., Díaz Palencia J.L., Wang N., Jiang Y., Wang D.-Y. *Nanocarbon-based flame retardant polymer nanocomposites*. **MOLECULES 26**, 2021.

102. Chen X., Yusuf A., del Rio J.S., Wang D.-Y. *A facile and robust route to polyvinyl alcohol-based triboelectric nanogenerator containing flame-retardant polyelectrolyte with improved output performance and fire safety*. **NANO ENERGY 81**, 2021.

103. Díaz-Núñez P., Thomä S.L.J., González-Rubio G., Borrell-Grueiro O., Höller R.P.M., Chanana M., Garoz D., Bañares L., Junquera E., Guerrero-Martínez A., Rivera A., Peña-Rodríguez O. *Rod-sphere cluster irradiation with femtosecond laser pulses: Cut and paste at the nanoscale*. **NANOPHOTONICS 10**, 3153-3159, 2021.

104. Fu C., Xu B., Dong L., Zhai J., Wang X., Wang D.-Y. *Highly efficient BiVO4 single-crystal nanosheets with dual modification: Phosphorus doping and selective Ag modification*. **NANOTECHNOLOGY 32**, 2021.

105. Macía E., García-Junceda A., Serrano M., Hong S.J., Campos M. *Effect of mechanical alloying on the microstructural evolution of a ferritic ODS steel with (Y–Ti–Al–Zr) addition processed by Spark Plasma Sintering (SPS)*. **NUCLEAR ENGINEERING AND TECHNOLOGY 53**, 2582-2590, 2021.

106. Bitarafan M.H., Zhou S., Hänninen J., Duan Y., Leino M., Ras R.H.A., Toivonen J. L*ight-patterned fluorescent gold nanoclusters in polycarbonate films*. **OPTICAL MATERIALS EXPRESS 11**, 4015-4025, 2021.

107. Martínez-Alonso C., Guevara-Vela J.M., LLorca J. *The effect of elastic strains on the adsorption energy of H, O, and OH in transition metals*. **PHYSICAL CHEMISTRY CHEMICAL PHYSICS 23**, 21295-21306, 2021.

108. Fu C., Ye W., Zhai Z., Zhang J., Li P., Xu B., Li X., Gao F., Zhai J., Wang D.-Y. *Self-cleaning cotton fabrics with good flame retardancy via one-pot approach*. **POLYMER DEGRADATION AND STABILITY 192**, 2021.

109. Liu W., Pan Y.-T., Zhang J., Zhang L., Moya J.S., Cabal B., Wang D.-Y. *Low-melting phosphate glasses as flame-retardant synergists to epoxy: Barrier effects vs flame retardancy*. **POLYMER DEGRADATION AND STABILITY 185**, 2021.

110. Rui W., Wenqing W., Fanghe W., Anying Z., Xiuqin Z., Deyi W. *Construction of nano-multilayer coatings on copolyester fabrics using UV-grafting mediated layer-by-layer self-assembly for improved anti-droplet and flame retardent performance*. **POLYMER DEGRADATION AND STABILITY 183**, 2021.

111. Lin S., Tao B., Zhao X., Chen G., Wang D.-Y. *Surface functionalization of black phosphorus via amine compounds and its impacts on the flame retardancy and thermal decomposition behaviors of epoxy resin*. **POLYMERS 13**, 2021.

112. Gibney R., Patterson J., Ferraris E. *High-resolution bioprinting of recombinant human collagen type iii*. **POLYMERS 13**, 2021.

113. Omar H., Smales G.J., Henning S., Li Z., Wang D.-Y., Schönhals A., Szymoniak P. Calorimetric and dielectric investigations of epoxy-based nanocomposites with halloysite nanotubes as nanofillers. POLYMERS 13, 2021.

114. Yang Y., Wang D.-Y., Haurie L., Liu Z., Zhang L. *Combination of corn pith fiber and biobased flame retardant: A novel method toward flame retardancy, thermal stability, and mechanical properties of polylactide*. **POLYMERS 13**, 2021.

115. Pascual-González C., Thompson C., de la Vega J., Biurrun Churruca N., Fernández-Blázquez J.P., Lizarralde I., Herráez-Molinero D., González C., LLorca J. *Processing and properties of PLA/Mg filaments for 3D printing of scaffolds for biomedical applications*. **RAPID PROTOTYPING JOURNAL** , 2021.

116. EzEldeen M., Toprakhisar B., Murgia D., Smisdom N., Deschaume O., Bartic C., Van Oosterwyck H., Pereira R.V.S., Opdenakker G., Lambrichts I., Bronckaers A., Jacobs R., Patterson J. *Chlorite oxidized oxyamylose differentially influences the microstructure of fibrin and self assembling peptide hydrogels as well as dental pulp stem cell behavior*. **SCIENTIFIC REPORTS 11**, 2021.

117. Jacobo-Martín A., Rueda M., Hernández J.J., Navarro-Baena I., Monclús M.A., Molina-Aldareguia J. M., Rodríguez I. *Bioinspired antireflective flexible films with optimized mechanical resistance fabricated by roll to roll thermal nanoimprint*. **SCIENTIFIC REPORTS 11**, 2021.

118. Krishnapriyan A.S., Montoya J., Haranczyk M., Hummelshøj J., Morozov D. *Machine learning with persistent homology and chemical word embeddings improves prediction accuracy and interpretability in metal-organic frameworks*. **SCIENTIFIC REPORTS 11**, 2021.

119. Banait S., Jin X., Campos M., Pérez-Prado M.T. *Precipitation-induced transition in the mechanical behavior of 3D printed Inconel 718 bcc lattices*. **SCRIPTA MATERIALIA 203**, 2021.

120. Sapanathan T., Sabirov I., Xia P., Monclús M.A., Molina-Aldareguía J. M., Jacques P.J., Simar A. *High temperature in situ SEM assessment followed by ex situ AFM and EBSD investigation of the nucleation and early growth stages of Fe-Al intermetallics*. **SCRIPTA MATERIALIA 200**, 2021.

121. Sánchez del Río J., Pascual-González C., Martínez V., Jiménez J.L., González C. *3D-printed resistive carbon-fiber-reinforced sensors for monitoring the resin frontal flow during composite manufacturing*. **SENSORS AND ACTUATORS, A: PHYSICAL 317**, 2021.

122. Pou-Álvarez P., Riveiro A., Nóvoa X.R., Jin X., del Val J., Comesaña R., Boutinguiza M., Lusquiños F., Jones J.R., Pérez-Prado M.T., Pou J. *Laser-Guided Corrosion Control: A New Approach to Tailor the Degradation of Mg-Alloys*. **SMALL 17**, 2021.

123. Szymoniak P., Qu X., Abbasi M., Pauw B.R., Henning S., Li Z., Wang D.-Y., Schick C., Saalwächter K., Schönhals A. *Spatial inhomogeneity, interfaces and complex vitrification kinetics in a network forming nanocomposite*. **SOFT MATTER 17**, 2775-2790, 2021.

124. Mendez A., Monclus M.A., Santiago J.A., Fernandez-Martinez I., Rojas T.C., Garcia-Molleja J., Avella M., Dams N., Panizo-Laiz M., Molina-Aldareguia J. M. *Effect of Al content on the hardness and thermal stability study of AlTiN and AlTiBN coatings deposited by HiPIMS*. **SURFACE AND COATINGS TECHNOLOGY 422**, 2021.

125. Lopez-Cabanas I., LLorca J., González-Arrabal R., Meletis E.I., Molina-Aldareguia J. M. *High throughput optimization of hard and tough TiN/Ni nanocomposite coatings by reactive magnetron sputter deposition*. **SURFACE AND COATINGS TECHNOLOGY 418**, 2021.

3.2. Book chapters

1. T. Meštrović, J. Patterson. *Human Microbiome and Disease*. In **Reference Module in Biomedical Sciences,** 2021.

2. P. Alvaredo, J. M. Torralba, A. García-Junceda*. Sintering of High Entropy Alloys: Processing and Properties*. In **Encyclopedia of Materials: Metals and Alloys,** 362-371, 2021.

3. M. Campos, J. M. Torralba, R. Casas, M. Carton-Cordero*. Sintering of Superalloys: Processing and Properties.* In **Encyclopedia of Materials: Metals and Alloys,** 372-382, 2021.

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 Technical University of Madrid. Patent application number P202131218 (28 December 2021)

3.4. International conferences. Invited and plenary talks

1. *"Functionalized nano-hybrids as new generation flame retardants to improve the fire safety of polymers for advanced application"*, D-Y Wang, **Webinar on Energy Materials and Technologies**, Virtual, Singapore, January 2021.
2. *"Novel Variational Formulations for the Solution of Coupled Problems and Inelastic Structures"*, I. Romero, **14th World Congress on Computational Mechanics (WCCM14)**, Paris, France, January 2021.
3. *"Integrated Models for the Design of Precipitation Hardenable Mg and Al Alloys"*, H. Liu, I. Papadimitriou, F-X. Lin, J. LLorca, J-F Nie, N. Moelans, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
4. *"Strength and fracture toughness of monolithic and multilayered hard coatings"*, J. M. Molina-Aldareguia, **International Conference on Metallurgical Coatings and Thin Films 2021 (ICMCTF 2021)**, Virtual, April 2021.
5. *"Metallic powders for Additive Manufacturing"*, J. M. Torralba, **INVIRTA Workshops**, Baviera, Germany, April 2021.
6. *"Additive manufacturing of High Entropy Alloys"*, J. M. Torralba, **INVIRTA Workshops**, Baviera, Germany, May 2021.
7. *"Fundamental research and industrial application of flame retardant"*, D-Y Wang, **NFRTI 4th National Forum on Flame-retardant Industrailization and Technological Innovation** , Shanghai, China, May 2021.
8. *"High-performance materials based on nanoscopic building blocks from composites to electrodes. NT21"*, J. J. Vilatela, **3rd Symposium on Nanocarbon Materials for Energy and Sustainability**, Houston (Texas), USA, June 2021.
9. *"Crack Propagation in metal-ceramic and metal-metal nanolaminates"*, J. M. Molina-Aldareguia, **6th International Virtual Conference of Engineering Against Failure (ICEAF VI)**, Virtual, June 2021.
10. *"Computational Metallurgy"*, D. Tourret, **CNRS Summer School on Solidification**, Virtual, June 2021.
11. *"Alloying effects on the CRSS for slip and twinning Mg alloys: a high- throughput investigation based on diffusion couples"*, J. M. Molina-Aldareguia, **E-MRS Spring Meeting**, Virtual, June 2021.
12. *"Dislocation-particle Interactions in Magnesium Alloys"*, M. T. Perez-Prado, **12th International Conference on Magnesium alloys and their applications (Mg2021)**, Montreal, Canada, June 2021.
13. *"Effect of solutes and precipitates on slip activity in magnesium alloys"*, C. M. Cepeda-Jiménez, D. Shi, C. Wang, X. Jin, M. T. Pérez-Prado, **International Conference on Processing & Manufacturing of Advanced Materials: Processing, Fabrication, Properties, Applications (THERMEC'2021)** , Graz, Austria, June 2021.

14. *“Computational and data-driven approaches to smartly engineered porous materials”*, M. Haranczyk, **La Inteligencia Artificial en el descubrimiento de materiales inteligentes y en la mejora de procesos en la industria química** , Virtual, July 2021.
15. *“Modeling of microstructure development during fusion-based metal additive manufacturing “*, D. Tourret , **EUROMECH Colloquium on Microstructures and Micromechanisms in Metal Additive Manufacturing**, Virtual, July 2021.
16. *“Icosahedral quasicrystal-enhanced nucleation in Al alloys manufactured by selective laser melting”*, M. T. Pérez-Prado, **EUROMECH Colloquium on “Microstructures and micromechanisms in metallic additive manufacturing**, Palaiseau, France, July 2021.
17. *“Interaction between twin boundaries and precipitates at the atomic scale”*, D. Shi, C. Wang, C. M. Cepeda-Jiménez, M. T. Pérez-Prado, **Predictive Integrated Structural Materials Science (PRISMS)** , Virtual, August 2021.
18. *“Computational and data-driven approaches to smartly engineered porous materials “*, M. Haranczyk, **Smartly Engineered Materials for Energy and Environment**, Virtual, August 2021.
19. *“High entropy alloys obtained by Powder Mtallurgy”*, J. M. Torralba, **10th Global Conference on Materials Science and Engineering (CSE)**, Virtual, August 2021.
20. *“Modeling size effects in metals using FFT homogenization”*, J. Segurado, **2nd International Workshop on Plasticity, Damage and Fracture of Engineering Materials (IWPDF 2021)**, Ankara, Turkey, August 2021.
21. *“Nano-sized Flame Retardants: Structure, Properties and Mechanisms”*, D-Y Wang, **European Meeting on Fire Retardant Polymeric Materials (FRPM21)**, Budapest, Hungary, August/September 2021.
22. *“Development of a Cr-based hard composite processd by spark plasma sintering”*, J. M. Torralba, **3rd International Conference on Graphene and Novel Nanomaterials (GNN 2021)**, Virtual, August 2021.
23. *“Suspended 1D nanomaterials: synthesis via floating catalyst and direct assembly as high-performance network materials”*, J. J. Vilatela, **MRS Fall Meeting,** Virtual, September 2021.
24. *“Something more than powder”*, J. M. Torralba, **EUROMAT 2021**, Virtual, September 2021.
25. *“Structure and mechanics of continuous ensembles of carbon nanotubes: from bundles and nanoscale networks to macroscopic fabrics”*, J. J. Vilatela, **EUROMAT 2021**, Virtual, September 2021.
26. *“Coupling microstructure and mesostructure in Inconel 718 3D printed lattices”*, S. Banait, X. Jin, M. Campos, M. T. Pérez-Prado, **ITP Aero Technical Knowledge Days** Virtual, September 2021.
27. *“High strength magnesium alloys for sustainable transport”*, X. Jin, C. Wang, D. Shi, C. M. Cepeda-Jiménez, M. T. Pérez-Prado, **Virtual Congress and Exhibition of the German Materials Society**, Virtual, September 2021.
28. *“Gleeble Simulations for Manufacturing Process Improvements – Physical Simulations for Real Life Applications”*, I. Sabirov, **GLEEBLE webinar series** , New York, USA, September 2021.

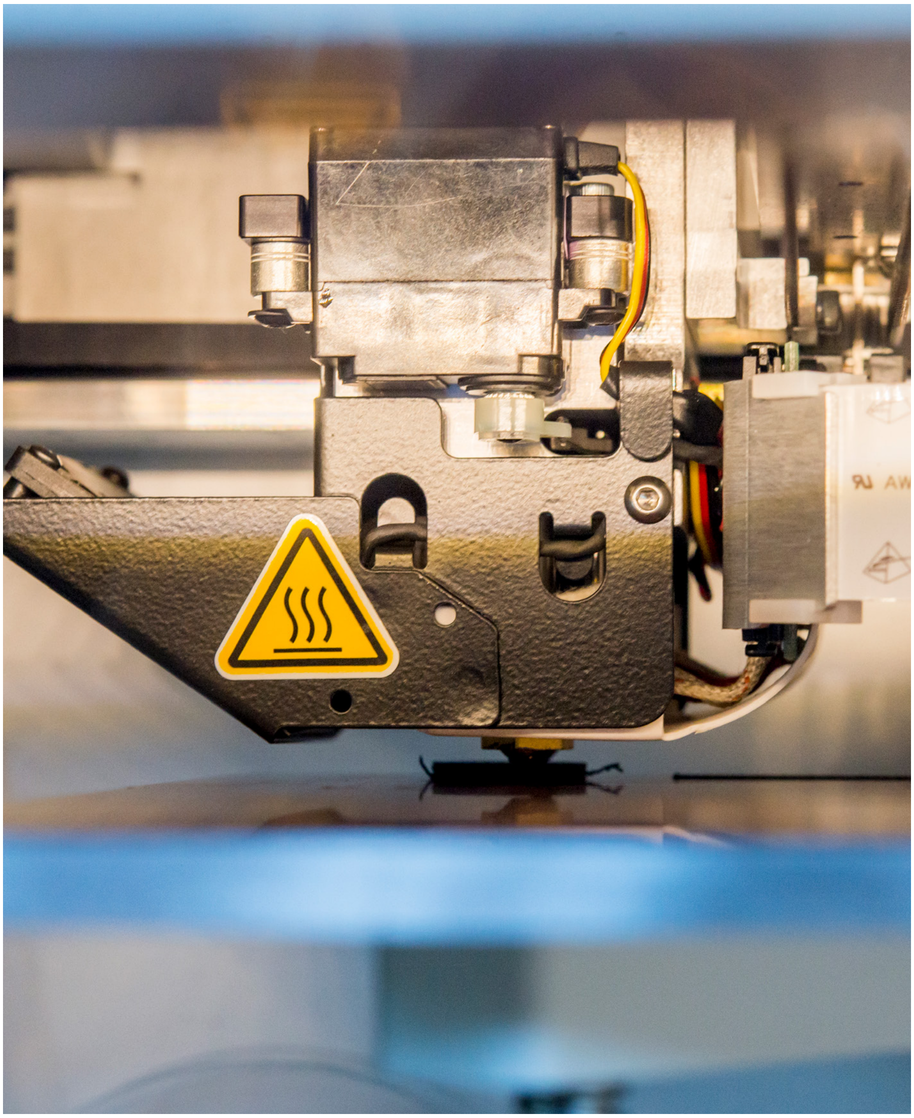
29. *"Dislocation dynamics prediction of the strength of Al-Cu alloys containing impenetrable (theta') and shearable (theta'') precipitates"*, R. Santos-Güemes, B. Bellón, J. Segurado, J. LLorca, **XVI International conference on Computational Plasticity (COMPLAS 2021)**, Barcelona, Spain, September 2021.
30. *"On the effect of slip transfer at grain boundaries on the strength and ductility of polycrystals"*, E. Nieto-Valeiras, S. Haouala, D. Barba, J. LLorca, **XVI International conference on Computational Plasticity (COMPLAS 2021)**, Barcelona, Spain, September 2021.
31. *"Coupling micro and mesostructure in Inconel 718 3D printed lattices"*, S. Banait, X. Jin, M. Campos, M. T. Pérez-Prado, **International Conference in Experimental and Computational Methods in Manufacturing (ICECMM2021),** Virtual, September 2021.
32. *"Some Progress in Flame Retardants"*, R. Yang, D-Y Wang, **1st China-Spain International Symposium on New Frontiers in Fire Safety Materials & Technologies,** Virtual, October 2021.
33. *"Spark plasma sintering consolidation of ceramics based on Portland clinker"*, J. M. Torralba, **1st Conference on FAST/SPS. From research to industry**, Poznan, Poland, October 2021.
34. *"Coupling microstructure and mesostructure in Inconel 718 3D printed lattices"*, S. Banait, X. Jin, M. Campos, M. T. Pérez-Prado, **International Conference on Additive Manufacturing (ICAM 2021)**, California, USA, November 2021.
35. *"Status and Prospect of Al alloys for Additive Manufacturing"*, S. Milenkovic, **26th International Conference on Advanced Materials & Nanotechnology**, Madrid, Spain, November 2021.
36. *"Advanced powder metallurgy to develop mass production parts, unique materials and outstanding materials"*, J. M. Torralba, **Symposium on Innovation in Materials Processing (ISIMP 2021)**, Jeju-do, South Korea, November 2021.

3.5. International conferences. Regular contributions

1. *"Thermally Reversible Bistable Metamaterials: A Theoretical Investigation Based on Singularity Theory"*, A. Vasudevan, J. Rodríguez-Martínez, I. Romero, **14th World Congress on Computational Mechanics (WCCM14)**, Paris, France, January 2021.
2. *"Structure-Preserving Integration of Molecular Dynamics"*, M. Schiebl, I. Romero, **14th World Congress on Computational Mechanics**, Paris, France, January 2021.
3. *"High energy/power density lithium-ion batteries through interface engineered CoO@3DNRGO pseudocapacitive anodes"*, V. S. Avvaru, V. Etacheri, **4th Erwin Schrödinger Symposium 2021 of the Erwin Schrödinger Society for Nanosciences**, Virtual, January 2021.
4. *"Unusual Pseudocapacitive Lithium Ion Storage Triggered by Nanograin Boundaries of Conversion Type Anodes Pseudocapacitive Lithium Ion Storage Triggered by*

Nanograin Boundaries of Conversion Type Anodes", V. S. Avvaru, V. Etacheri, **Swiss Battery days 2020/2021**, Zurich, Switerland, February 2021.

5. *"Interface engineered CoO@3D-NRGO pseudocapacitive anodes for high energy/power density lithium-ion batteries"*, V. S. Avvaru, V. Etacheri, **I Congreso Anual de Estudiantes de Doctorado**, Virtual, February 2021.
6. *"Dendritic spacing selection during Al-Cu casting: experiments and multiscale simulations"*, B. Bellón, A. Boukellal, T. Isensee, J. Coleman, M. Krane, M. Titus, D. Tourret, J. LLorca, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.



7. *"Grain boundary slip transfer classification and metric selection with artificial neural networks"*, Z. Zhao, T. Bieler, J. LLorca, P. Eisenlohr, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
8. *"Mechanical properties and biodegradability of porous Mg and Zn scaffolds fabricated by power bed laser fusion for biomedical applications"*, M. Li, F. Benn, T. Derra, A. Kopp, J. M. Molina-Aldareguia, J. LLorca, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
9. *"Mechanical properties and biodegradability of porous PLA/Mg and PLA/Zn scaffolds fabricated by fused filament deposition for biomedical applications"*, C. Pascual, C. Thompson, J. de la Vega, D-Y Wang, C. González, J. LLorca, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
10. *"First principles study of precipitation in Al-Cu, Al-Li and Al-Cu-Li alloys"*, S. Liu, J. LLorca, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
11. *"High-throughput experimental techniques to measure the CRSS for slip and twinning in Mg and Mg alloys"*, J. Wang, R. Alizadeh, J. LLorca, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
12. *"Simulation of the effect of corrosion on the mechanical properties of porous Mg scaffolds fabricated by power bed laser fusion for biomedical applications"*, M. Marvi-Mashhadi, M. Li, W. Ali, C. González, J. LLorca, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
13. *"Experimental analysis and numerical simulation of cyclic deformation and fFatigue behavior of AZ31 Mg alloy"*, A. Jamali, M. Zhang, A. Ma, J. LLorca, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
14. *"Accelerating development of promising nanocatalyzers assisted by statistical machine learning"*, G. Lo Dico, S. Croubels, V. Carcelén, M. Haranczyk , **2nd Webinar on Catalysis & Chemical Engineering** , Virtual, March 2021.
15. *"Multiscale Modeling of Dendritic Growth in Directional Solidification with Buoyant Flow"*, T. Isensee, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
16. *"Facetted growth in isothermal solidification of silicon: 3D phase-field simulations of growth and equilibrium shapes"*, A. K. Boukellal, **TMS 2021 Annual Meeting & Exhibition (TMS 2021)**, Virtual, March 2021.
17. *"Ultrahigh energy and power density batteries enabled by nanograin-boundary induced pseudocapacitive Li-ion storage"*, V. S. Avvaru, V. Etacheri, **World Nano Congress on Advanced Science and Technology (WNCST 2021)**, Vellore, India, March 2021.
18. *"Effect of solutes and precipitates on slip activity in magnesium alloys"*, C. M. Cepeda-Jiménez, D. Shi, C. Wang, X. Jin, M. T. Pérez-Prado, **Magnitogorsk Materials Week Conference in memory of Dr. Alexander Zhilyaev**, Virtual, April 2021.
19. *"Study of the generation and evolution of damage in NCF laminates subjected to thermalcycling"*, I. Lizarralde, E. Sapountzi, F. Sket, C. Gonzalez, **10th International**

Conference on Composite Testing and Model Identification (CompTest 2021), Virtual, May 2021.

20. *"Cyclic deformation mechanisms and fatigue life prediction of AZ31 Mg alloy. Mg 2021"*, A. Jamali, M. Zhang, A. Ma, J. LLorca, **12th International Conference on Mg alloys and its Applications (Mg2021)**, Virtual, June 2021.
21. *"Understanding the poor hardening potential of nanoprecipitates in highly alloyed magnesium rare earth alloys"*, X. Z. Jin, W. C. Xu, D. B. Shan, B. Guo, B. Jin, M. T. Pérez-Prado, **12th International Conference on Magnesium alloys and their applications (Mg2021)**, Virtual, June 2021.
22. *"Computer-aided detoxifier material design for animal feed "*, G. Lo Dico, S. Croubels, V. Carcelén, M. Haranczyk, **15th International conference on materials chemistry (MC15)**, Virtual, July 2021.
23. *"An FFT framework for simulating non-local ductile failure in heterogeneous materials"*, J. Segurado , **IUTAM Symposium - Generalized continua emerging from microstructures Dates**, Paris, France, July .
24. *"Multiscale prediction of primary dendritic spacing in metal alloy casting"*, B. Bellón, A. K. Boukellal, T. Isensee, O. M. Wellborn, K. P. Trumble, M. J. M. Krane, M. S. Titus, D. Tourret, J. LLorca, **EUROMAT 2021,** Virtual, September 2021.
25. *"Phase-field study of microstructure selection in hcp Mg alloys"*, A. K. Boukellal, M. Sarebanzadeh, A. Orozo-Caballero, J. LLorca, D. Tourret, **EUROMAT 2021,** Virtual, September 2021.
26. *"Machine-learning-aided design "*, G. Lo Dico, S. Croubels, V. Carcelén, M. Haranczyk, **MRS Fall meeting**, Virtual, September 2021.
27. *"A deep encoder-decoder network for surrogate modelling of liquid moulding of composites"*, J. Fernández, K. Keramati, L. Baumela, C. González, **Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology**, Virtual, September 2021.
28. *"Machine learning model to predict the type and properties of race-tracking during the liquid composite moulding in manfacturing process"*, K. Keramati, J. Fernández, C. González, **Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology**, Virtual, September 2021.
29. *"Data Driven ultrasonic NDT for porosity estimation in composite materials"*, Juan I. Caballero, C. González, C. Gonzalo, E. Menasalvas, F. Sket, **Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology**, Virtual, September 2021.
30. *"Characterization of an ultrafine eutectic Ti-Fe-based alloy processed by additive manufacturing via Near-Field Ptychographic Tomography"*, J. C. da Silva, P. Barriobero Vila, K. Bugelnig, U. Hecht, J. Gussone, P. Cloetens, F. Sket, J. Haubrich, G. Requena, **Nanoinnovation 2021 conference & exhibition**, Rome, Italy, September 2021.
31. *"Multiscale prediction of primary dendritic spacing in metal alloy casting"*, D. Tourret , **EUROMAT 2021**, Virtual, September 2021.

32. *"Multiscale Modeling of Dendritic Growth in Directional Solidification with Buoyant Flow"*, T. Isensee, **EUROMAT 2021**, Virtual, September 2021.
33. *"Multiscale Simulation of Melt Pool Solidification in Additive Manufacturing of Nickel-based Superalloys"*, R. Tavakoli, **EUROMAT 2021**, Virtual, September 2021.
34. *"Phase-field study of microstructure selection in hcp Mg alloys"*, A. K. Boukellal, **EUROMAT 2021**, Virtual, September 2021.
35. *"Thermal stability of nanostructure TiAl(B9N coatings deposited by HiPIMS"*, A.. Méndez, M. Monclús, I. Fernández, J. Antonio Santiago, J. M. Molina-Aldareguia, **EUROMAT 2021**, Virtual, September 2021.
36. *"Mechanical properties and biodegradability of porous Mg scaffolds fabricated by powder bed laser fusion for biomedical applications"*, M. Li, T. Derra, A. Kopp, N. Kroeger, Max Zinser, R. Smeets, J. LLorca, J. M. Molina-Aldareguia, **EUROMAT 2021**, Virtual, September 2021.
37. *"Data-driven ultrasonic NDT for porosity estimation in composite materials"*, J.I. Caballero, C. Gonzalez, E. Menasalvas, C. Gonzalo Martin, F. Sket, **Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology (MMLDT-CSET 2021)**, Virtual, September 2021.
38. *"Optimisation of SLM lattice structures of Inconel 718 for improving the mechanical behaviour"*, S. Banait, X. Jin, M. Campos, M. T. Pérez-Prado., **EuroPM2021**, Virtual, October 2021.
39. *"High performance Mg and Mg-Li/Na-ion hybrid batteries through defect engineering of metal oxide electrodes Vinodkumar Etacheri"*, V. Etacheri, M. Vincent, V. S. Avvaru, **7th International Congress on Energy Efficiency and Energy Related Materials (ENEFM2021)** , Mugla, Turkey, October 2021.
40. *"High performance Mg and Mg-Li/Na-ion hybrid batteries through defect engineering of metal oxide electrodes"*, V. Etacheri, M. Vincent, V. Sai Avvaru, **7th International Congress on Energy Efficiency and Energy Related Materials (ENEFM)**, Mugla, Turkey, October 2021.
41. *"Accelerating design of nanoporous catalyzers assisted by statistical machine learning"*, G. Lo Dico, V. Carcelén, M. Haranczyk , **RSC Catalysis Science & Technology 10th Anniversary Symposium**, Virtual, November 2021.
42. *"Resolution of Phase-Field Models By Means of FFT and GPU"*, A. Boccardo, **CHiMaD Phase-Field Workshop XII**, Virtual, November 2021.
43. *"A Julia GPU Parallelized Implementation of the Nucleation Benchmark"*, J. Mancias, **CHiMaD Phase-Field Workshop XII**, Virtual, November 2021.
44. *"Multiscale Modeling of Composites: Towards Artificial Intelligence Assisted Virtual Testing of Composites"*, M. Zarzoso, C. González, J. Vilatela, P. Romero-Rodríguez, **ECCOMAS Thematic CM3 Transport Workshop 2021**, Barcelona, Spain, November 2021.
45. *"Precipitation hardening in Al and Mg alloys"*, J. LLorca, **4th International Conference on Light Materials - Science and Technology Light MAT 2021**, Virtual, November 2021.

46. *"Machine-Learning-Accelerated Experimental Characterization and Multiobjective Design Optimization of Natural Porous Materials "*, G. Lo Dico, V. Carcelén, M. Haranczyk, **MRS Fall meeting,** Virtual, December 2021.

3.6. International conferences. Membership in organising committees

1. **European Meeting on Fire Retardant Polymeric Materials (FRPM21).** D-Y Wang (International scientific committee member). Budapest, Hungary, August 2021.
2. **EUROMAT 2021.** D. Tourret (Symposium Organiser). Virtual, September 2021.
3. **EUROMAT 2021.** J. J. Vilatela (Co-organiser). Virtual, September 2021.
4. **EUROMAT 2021.** J. M. Molina-Aldareguia (Symposium organizer). Virtual, September 2021.
5. **International Conference on Experimental and Computational Methods in Manufacturing (ICECMM 2021).** M. T. Pérez-Prado (Member of the International Advisory Committee), Nirjuli, India, September 2021.
6. **MRS Fall Meeting.** M. Haranczyk (Symposium co-organizer). Virtual, December 2021.
7. **TMS 2021 Annual Meeting & Exhibition (TMS 2021).** D. Tourret (Symposium Organiser), Virtual, March 2021.
8. **The 12th International Conference on Magnesium Alloys and their Applications (Mg2021).** M. T. Pérez-Prado (Member of the International Advisory Committee), Virtual, July 2021.

3.7. Invited seminars and lectures

1. *"High-throughput experimental techniques to measure the CRSS for slip and twinning in Mg and Mg alloys"*, J. LLorca, **Indian Institute of Technology Goa**, Goa, India, March 2021
2. *"The Use of Diffusion Couples and Micropillar Compression to Determine Alloying Effects On the CRSS for Slip and Twinning in Mg Alloys"*, J. M. Molina-Aldareguia, **Michigan State University**, Virtual, March 2021
3. *"Fracture behavior of metal-ceramic and metal-metal nanolaminates"*, J. M. Molina-Aldareguia, **Université de Lille**, Virtual, June 2021
4. *"High-performance materials based on nanoscopic building blocks: from composites to electrodes"*, J. J. Vilatela, **AIST**, Tokyo, Japan, July 2021
5. *"Ánodos de silicio para la nueva generación de baterías ion Litio: retos científicos y de industrialización"*, J. J. Vilatela, **Red mexicana de almacenamiento de energía**, Puebla, México, September 2021
6. *"High-performance materials based on nanoscopic building blocks: from composites to electrodes"*, J. J. Vilatela, **Chalmers University**, Gothenburg, Sweden, November 2021

7. *“Progress of fire retardant materials*”, D-Y Wang, **Henan University**, Kaifeng, China, November 2021
8. *“FFT based simulations for capturing microstructure effect on the mechanical response of metals*”, J. Segurado, **Webinar at IMDEA**, Madrid, Spain, November 2021
9. *“Metal additive manufacturing technology*”, S. Milenkovic, **Faculty of Technology and Metallurgy**, Belgrade, Serbia, December 2021

3.8. Awards

1. Outstanding Reviewer Award 2020, Acta & Scripta Materialia, **D. Tourret.**
2. Outstanding Key Reader Award 2020, Metallurgical & materials Transactions A, **D. Tourret.**
3. Award to the best doctoral thesis, Technical University of Madrid, 2021, **G. Esteban-Manzanares.**
4. European Materials Gold Medal 2021, Federation of European Materials Societies (FEMS), July 2021, **J. M. Torralba.**

3.9. Seminars

1. *“Microstructure-based plasticity of metals – Going from the atomic to the continuum scale”* **Prof. D. Mordehai** (from Tehnion Israel). April 2021
2. “*Metallic materials for biodegradable implants and antimicrobial surfaces”* **Dr. S.** Sánchez (from Northumbria University in UK). July 2021
3. *“Tailor-made nanostructured catalysts for photo- and electro-chemical energy conversion”* **Dr. H. Tüysüz** (from Max-Planck-Institut für Kohlenforschung in Germany). September 2021
4. *“Vibrant future for acoustic and mechanical metamaterials”* **Prof. J. Christensen** (from Carlos III University of Madrid). September 2021
5. *“Laser bioprinting from single cell to tissue engineering”* **Prof. C. Molpecere** (from the Technical University of Madrid). October 2021
6. *“The next technology to make aviation cleaner”* **J. Fernandez Castañeda** (from ITP Aero). October 2021
7. *“Nanoheterostructures based on wide bandgap semiconducting oxides: synthesis and optical properties”* **Prof. B. Mendez** (from the Complutense University of Madrid). November 2021

4. Technology offer

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

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

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

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

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

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

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

Title: 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 Homogenization Code, MADrid)
Description: FFT-based simulation tool developed by IMDEA Materials for computational homogenization of any heterogeneous material, such as composites, polycrystals or celular materials, by simulating the behavior of a Representative Volume Element of the microstructure.
Opportunity: Software License

Title: 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 homogenization simulation tools.
Opportunity: Software License

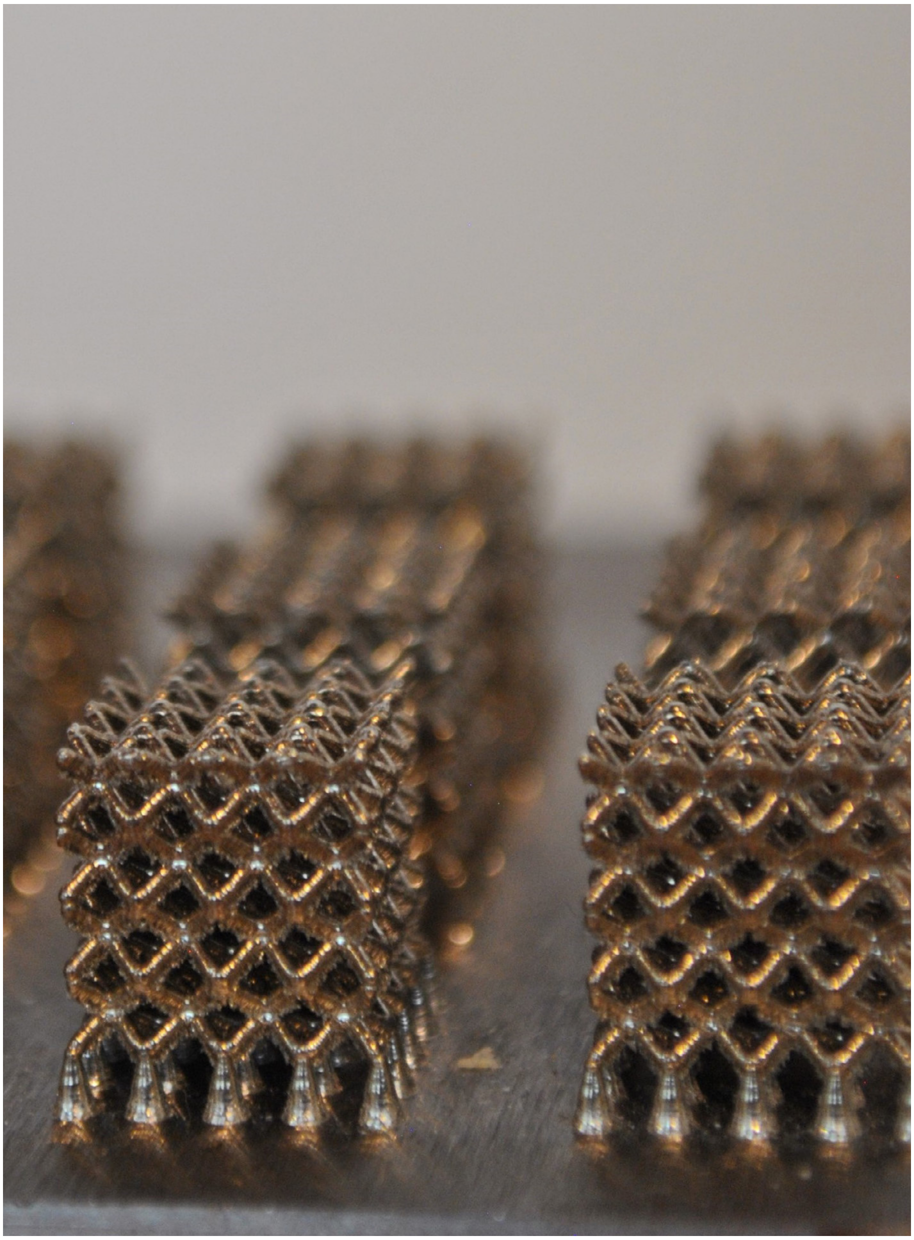
Title: MULTIFOAM
Description: Simulation tool developed within the framework of computational micromechanics by IMDEA Materials to predict the mechanical behavior of low to medium density foams with open and closed-cell microstructure
Opportunity: Software License

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

Title: MUESLI

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

Opportunity: Software License



5. Training, communication and outreach

5.1. Theses

PhD Theses

1. *"X-Ray Tomographic Investigation of Resin Flow in Liquid Moulding of Composite Materials"*
   Student: Jaime Castro Arias
   Advisor: Dr. F. Sket. Prof. C. González
   Date of defense: January 2021

2. *"Design and study of multifunctional fabrics"*
   Student: Can Fu
   Advisor: Dr. D. Wang
   Date of defense: December 2021

3. *"Metal organic frameworks (MOFs) derived hierarchically nanomaterials as multifunctional fire retardant for polymer nanocomposites"*
   Student: Jing Zhang
   Advisor: Dr. D. Wang
   Date of defense: January 2021

4. *"High performance flame retardant rigid polyurethane foam with high thermal insulation"*
   Student: Pablo Acuña Dominguez
   Advisor: Dr. D. Wang
   Date of defense: May 2021

5. *"Analysis of precipitation hardening in metallic alloys by means of dislocation dynamics"*
   Student: Rodrigo Santos Guemes
   Advisor: Prof. J. Llorca, Prof. J. Segurado
   Date of defense: June 2021

6. *"Towards mimicking the foetal liver niche: Engineering 3D hydrogel systems for in-vitro culture of hematopoietic stem cells"*
   Student: Christian Jose Garcia Abrego
   Advisor: Dr. J. Patterson, Dr. C. Verfaillie, Dr. C. Bartic
   Date of defense: September 2021

7. *"Experimental and computational micro-mechanics of fibre- reinforced polymer composites at high strain rate"*
   Student: Mario Rueda
   Advisor: Dr. J. Molina; Dr. B. Beake
   Date of defense: July 2021

8. *"Influence of Al and Zn alloying additions on the deformation mechanisms of Mg alloys"*
   Student: Dongfeng Shi
   Advisor: Dr. M. T. Pérez-Prado, Dr. C. M. Cepeda-Jiménez
   Date of defense: December 2021

9. *"Automated Discovery of porous molecular materials facilitated by characterization of molecular porosity"*
   Student: Ismael Gómez García
   Advisor: Dr. M. Haranczyk
   Date of defense: September 2021

10. *"Quest for high performance Mg ang Mg-Li/Na ion hybrid batteries"*
    Student: Mewin Vincent
    Advisor: Dr. V. Etacheri, Dr. M. Haranczyk
    Date of defense: October 2021

11. *"Nanoengineered Pseudocapacitive Anodes for Rechargeable"*
    Student: Rudi Rubén Maça Alaluf
    Advisor: Dr. V. Etacheri
    Date of defense: November 2021

12. *"Nanoscale Engineered Electrode Materials for High Performance Lithium-Ion Batteries"*
    Student: Venkata Sai Avvaru
    Advisor: Dr. V. Etacheri
    Date of defense: October 2021

13. *"Na-ion Hybrid Energy Storage Devices Based on Nanengineered Electrodes"*
    Student: Wenliang Feng
    Advisor: Dr. V. Etacheri
    Date of defense: September 2021

Theses. Master/Bachelor Theses

1. *"Development of novel bio-based phase change materials for thermal"*
   Student: Alba Marta López González
   Carlos III University of Madrid
   Advisor: Dr. D-Y Wang
   Date of defense: September 2021

2. *"Transmisión de pulsos de autogeneradores TENG mediante protocolo LoRaWAN"*
   Student: Ignacio Astarloa Olaizola
   ICAI Comillas University
   Advisor: Dr. D-Y Wang
   Date of defense: May 2021

3. *"High performance fire retardant polymers"synthesis, characterization and properties"*
   Student: Eduardo Domínguez Ruiz
   Technical University of Madrid
   Advisor: Dr. D-Y Wang
   Date of defense: January 2021

4. *"Análisis en frecuencia de una señal generada por un autogenerador de energía TENG"*
   Student: Lucía Urbelz López-Puertas
   ICAI Comillas University
   Advisor: Dr. D-Y Wang
   Date of defense: July 2021

5. *"Determination of the fracture energy of fiber-matrix interface based on finite element advanced simulations of micromechanical models with experimental validation"*
   Student: José Manuel Camacho Serrano
   Technical University of Madrid
   Advisor: Dr. D. Garoz
   Date of defense: July 2021

6. *"Fabricación, caracterización mecánica de materiales compuestos reforzados con interleaves de nanotubos, fractura interlaminar"*
   Student: Jorge Naranjo Robles
   Technical University of Madrid
   Advisor: Dr. Y. Ou
   Date of defense: July 2021

7. *"Deformation behaviour of a novel Ni-based superalloy processed via spark plasma sintering"*
   Student: Antonio Potenciano Carpintero
   Carlos III University of Madrid
   Advisor: Dr. I. Sabirov, Prof. J. M. Torralba
   Date of defense: September 2021

8. *"Additive manufacturing of porous PLA/Mg and PLA/Zn scaffolds for biomedical applications"*
   Student: Diego Herráez Molinero
   Technical University of Madrid
   Advisor: Dr. C. Pascual
   Date of defense: July 2021

9. *"Relación entre la microestructura y el endurezamiento por deformación de una aleación "-TiAl a diferentes temperaturas"*
   Student: Berta Ruiz Palenzuela
   Carlos III University of Madrid
   Advisor: Dr. I. Sabirov, Prof. E. M. Ruiz-Navas
   Date of defense: September 2021

10. *"Degradation and biological evaluation of biodegradable composites of PLA/Mg manufactured by 3D printing for bone regeneration scaffold"*
Student: Martín Pedriza Herrero
Technical University of Madrid
Advisor: Dr. M. Echeverry-Rendón
Date of defense: July 2021

11. *"Characterization Of Hydrogel Formulations For Bioprinting And Tissue Engineering"*
Student: Ángela Castro María
Complutense University of Madrid
Advisor: Dr. J. Patterson
Date of defense: March 2021

12. *"Experimental analysis of the processing-microstructure link in Ni alloys manufactured by selective laser melting"*
Student: Patricia Caño Rebollar
Technical University of Madrid
Advisor: C. Galera
Date of defense: January 2021

13. *"Diseño y fabricación de un cabezal de impresión aditiva para ingeniería de tejidos"*
Student: Carlos López Torrado
Technical University of Madrid
Advisor: Dr. J.Patterson
Date of defense: September 2021

14. *"Piezoresistive properties of nanostructured networks"*
Student: Ángel Víctor Labordet Álvarez
Carlos III University of Madrid
Advisor: Dr. J. J.Vilatela
Date of defense: July 2021

15. *"Development and characterization of new silicon nanowires based electrodes for lithium ion batteries. (defiende en abril21)"*
Student: Joaquim Gispert Montserrat
Ramón Llul University
Advisor: Dr. J. J. Vilatela
Date of defense: July 2021

5.2. Internships / Visiting students

1. *"Multifunctional phase change materials (PCMs) for intelligent electronic devices"*
Student: Alba Marta López
Advisor: Dr. D-Y Wang
Visiting student from: Carlos III University of Madrid
Period: June 2021 - December 2021

2. *"High Performance Polymer Nanocomposites"*
Student: Antonio del Bosque
Advisor: Dr. D-Y Wang
Visiting student from: European University of Madrid
Period: September 2021 - December 2021

3. *"Multiscale characterization of advanced material "*
Student: Daniel Hernández
Advisor: Dr. F. Sket
Visiting student from: InTalentia
Period: June 2021 - September 2021

4. *"Martensitic stainless steels via quenching and partitioning process "*
Student: Berta Ruiz
Advisor: Dr. I. Sabirov
Visiting student from: InTalentia
Period: October 2020 - June 2021

5. *"Biological performance of degradable metals nanoparticles generated by spark discharge"*
   Student: Carmen Suriñe Zalbidea
   Advisor: Prof. J. LLorca; Dr. M. Echeverry-Rendón
   Visiting student from: InTalentia
   Period: September 2021 - December 2021

6. *"Development of machine learning algorithms to predict the processing-microstructure link during additive manufacturing"*
   Student: Patricia Caño
   Advisor: Prof. J. Llorca; Dr. G. Esteban
   Visiting student from: Technical University of Madrid
   Period: October 2020 - July 2021

7. *"Fabricación aditiva de materiales biodegradables para aplicaciones biomédicas"*
   Student: Sara Comeron
   Advisor: Prof. J. LLorca
   Visiting student from: Fundación Dádoris
   Period: July 2021 - July 2021

8. *"Estudio de la deformación y fractura de mecanismos de aleaciones Mg"*
   Student: Biaobiao Yang
   Advisor: Prof. J. LLorca
   Visiting student from: Technical University of Madrid
   Period: December 2021 - November 2022

9. *"(Sabbatical)"*
   Student: Dan Mordehai
   Advisor: Prof. J. LLorca
   Visiting scientist from: Technion
   Period: April 2021 - July 2021

10. *"VirtualBats project"*
    Student: Eduardo Roque
    Advisor: Prof. J. Segurado
    Visiting student from: Loyola University
    Period: September 2021 - October 2021

11. *"Synthesis and physicochemical characterization of low molecular weight gelatin (LMWG) hydrogels for 3D bioprinting"*
    Student: Álvaro Rojo
    Advisor: Dr. J. Patterson
    Visiting student from: Carlos III University of Madrid
    Period: December 2021 - Unfinished

12. *"Characterization Of Hydrogel Formulations For Bioprinting And Tissue Engineering"*
    Student: Ángela Castro
    Advisor: Dr. J. Patterson
    Visiting student from: Complutense University of Madrid
    Period: January 2021 - June 2021

13. *"Comparison of chemically versus physically crosslinked hydrogels as tissue engineering scaffolds"*
    Student: Beatriz Leiva
    Advisor: Dr. J. Patterson
    Visiting student from: InTalentia
    Period: July 2021 - August 2021

14. *"Synthesis and physicochemical characterization of low molecular weight gelatin (LMWG) hydrogels for 3D bioprinting"*
    Student: Claudia Montoro
    Advisor: Dr. J. Patterson
    Visiting student from: Carlos III University of Madrid
    Period: November 2021 - Unfinished

15. *"Comparison of chemically versus physically crosslinked hydrogels as tissue engineering scaffolds"*
    Student: Miguel Sánchez
    Advisor: Dr. J. Patterson
    Visiting student from: Technical University of Madrid
    Period: June 2021 - July 2021

16. *"Characterization of the mechanical properties of the fiber-matrix interface in composite laminates via nano- and micro-mechanical tests combined with advanced simulations"*
Student: Jorge Hernández
Advisor: Dr. J. M. Molina-Aldareguia
Visiting student from: Carlos III University of Madrid
Period: December 2020 - October 2021

17. *"Materials mechanics"*
Student: Alberto Orozco
Advisor: Dr. J. M. Molina-Aldareguia
Visiting student from: Technical University of Madrid
Period: July 2019 - Unfinished

18. *"Hard Coatings"*
Student: Álvaro Méndez
Advisor: Dr. J. M. Molina-Aldareguia
Visiting student from: Nano4Energy
Period: January 2019 - Unfinished

19. *"Online monitoring of SLM processes"*
Student: Giovanni Ortiz
Advisor: Dr. J. M. Molina-Aldareguia
Visiting student from: Technical University of Madrid
Period: June 2020 - Unfinished

20. *"Enhanced plasticity of a flash sintered binderless tungsten carbide"*
Student: Isacco Mazo
Advisor: Dr. J. M. Molina-Aldareguia
Visiting student from: University of Trento
Period: June 2021 - Unfinished

21. *"Participación en proyectos de investigación científica"*
Student: Alexandro Radita
Advisor: Prof. J. M. Torralba
Visiting student from: Fundación Dádoris
Period: July 2021 - July 2021

22. *"Improvement of interfacial properties of carbon nanotube fibres"*
Student: Daniel Iglesias
Advisor: Dr. J. J. Vilatela
Visiting student from: Trieste University
Period: February 2017 - March 2017

23. *"Estudio sobre la fabricación y propiedades de fotoánodos mesoporosos de óxido de titanio"*
Student: Isabel Gómez
Advisor: Dr. J. J. Vilatela
Visiting student from: Technical University of Madrid
Period: May 2021 - Unfinished

24. *"Nanostructured networks for high-power battery electrodes"*
Student: Carolina Ramos
Advisor: Dr. J. J. Vilatela
Visiting student from: InTalentia
Period: June 2021 - August 2021

25. *"Mejora de propiedades intermoleculares en fibras de CNTs mediante métodos de densificación"*
Student: David Luengo
Advisor: Dr. J. J. Vilatela
Visiting student from: Technical University of Madrid
Period: October 2020 - September 2021

26. *"Influence of ZrH2 quantity as well as the influence of the heat treatment on the granular structure of an L-PBF Al7075 alloy"*
Student: Nicolas Nothomb
Advisor: Dr. M. T. Pérez-Prado
Visiting student from: Louvain University
Period: November 2021 - December 2021

27. *"Improvement of the 3D Metal Jet Part Quality through print mode development supported by the HR-XCT characterization of the printed parts"*
Student: Sergi Bafaluy
Advisor: Dr. M. T. Pérez-Prado
Visiting student from: HP Printing and Computing Solutions - Carlos III University of Madrid
Period: January 2020 - Unfinished

28. *"Modeling adsorption in special clays"*
Student: Giulia Lo Dico
Advisor: Dr. M. Haranczyk
Visiting student from: University of Palermo
Period: March 2019 - Unfinished

29. *"Computational discovery of nanoporous materials for various energy applications"*
Student: Diego Martínez
Advisor: Dr. M. Haranczyk
Visiting student from: Technical University of Madrid
Period: June 2021 - July 2021

30. *"Desarrollo de algoritmos enfocados a tareas específicas"*
Student: Jorge Zorrilla
Advisor: Dr. M. Haranczyk
Visiting student from: Carlos III University of Madrid and Santiago de Compostela University
Period: September 2021 - Unfinished

31. *"Desarrollo de algoritmos enfocados a tareas específicas"*
Student: Lucas Perea
Advisor: Dr. M. Haranczyk
Visiting student from: Carlos III University of Madrid and Santiago de Compostela University
Period: July 2021 - Unfinished

5.3. Teaching in Masters

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

2. *"Advanced Composite Materials"*
Carlos III University of Madrid,
Professor: Dr. J. M. Molina-Aldareguia

3. *"Simulation in materials science and engineering"*
Carlos III University of Madrid,
Professor: Dr. J. M. Molina-Alderaguia

4. *"Simulation in materials materials engineering"*
Technical University of Madrid
Professor: Dr. D. Tourret

5. *"Simulation"*
Technical University of Madrid
Professor: Prof. C. González

6. *"Design and manufacturing of Advanced Composite Materials"*
Technical University of Madrid
Professor: Prof. C. González

7. *"Structural Characterization of Materials II: Spectroscopy"*
Technical University of Madrid
Professor: Dr. F. Sket

8. *"Advanced simulation methods"*
Technical University of Madrid
Professor: Prof. I. Romero

9. *"Advanced Numerical methods"*
Technical University of Madrid
Professor: Prof. J. Segurado

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

11. *"Nanomaterials"*
University of Navarra
Professor: Dr. J. J. Vilatela

12. *12. "Hierarchical Composites"*
Technical University of Madrid,
Professor: Dr. J. J. Vilatela

13. *"Additive Manufacturing"*
University of Navarra
Professor: Dra. M. T. Pérez

5.4. Institutional activities

1. *Member of the European Technology Platform for Advanced Engineering Materials and Technologies (EUMAT)*
2. *Member of the European Materials Characterization Council (EMCC)*
3. *Member of the European Aeronautics Science Network (EASN)*
4. *Member of the European Energy Research Alliance (EERA)*
5. *Member of the Batteries European Partnership Association (BEPA)*
6. *Member of the European Technology and Innovation Platform Batteries Europe*
7. *Member of the Royal Society of Chemistry*
8. *Member of the European Mechanics Society (EUROMECH)*
9. *Member of the Spanish Association of Composite Materials (AEMAC)*
10. *Technical Secretariat of the Spanish Technological Platform of Advanced Materials and Nanomaterials (MATERPLAT)*
11. *Member of the Spanish Aerospace 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 Ceramics and Glass Society (SECV)*
16. *Member of the Spanish Society of Numerical Methods in Engineering (SEMNI)*
17. *Member of the Spanish Materials Society (SOCIEMAT)*
18. *Member of the Spanish Society of Theoretical and Applied Mechanics (SEMTA)*
19. *Member of the Spanish Catalysis Society (SECAT)*
20. *Member of the Spanish Royal Society of Chemistry (RSEQ)*
21. *Member of the Madrid Aerospace Cluster (MAC)*
22. *Member of the Severo Ochoa Centres and María de Maetzu Units Alliance (SOMMA)*
23. *Local Contact Point of the EURAXESS network*
24. *Member of the Spanish Association of Foundations (AFE)*
25. *Member of the Network of Research Laboratories of Comunidad de Madrid (REDLAB)*

5.5. Individual participation in committees and other institutions

1. *Workshop: Preparing a Winning Application Package (TMS).* Dr. D. Tourret.

2. *Judging/evaluation for student (university level) scholarships, society level achievement awards, chapter awards, student conference abstracts and presentations (Society of Women Engineers), judging of student chapter award entries (Biomedical Engineering Society), judging of student business plan competition (Conrad Foundation), and judging for Student Research Showcase and chapter award entries (Sigma Xi). Dr. J. Patterson.*

3. *Volunteer mentor for Princeton University students (Princeton University).* Dr. J. Patterson.

4. *Member of Women in Academia Committee and Awards & Recognition Committee (Society of Women Engineers).* Dr. J. Patterson.

5. *Member of Board of Directors and Chair of the International Outreach Committee (Sigma Xi)* Dr. J. Patterson.

5.6. Outreach

1. *Organisation of the "2nd open PhD day" at IMDEA Materials. May 2021.*

2. *Organisation of the "15th Anniversary of the Multifunctional Nanocomposites Group". October 2021. J. J. Vilatela.*

3. *Participation in the "Science Week Madrid 2021. November 2021. C. Pereira, C. Pascual, A. del Bosque, A. Ma, L. Cobian, A. Fernández*

4. *Participation in the "European Researchers' night Madrid 2021 - What are you doing to improve the planet. November 2021. J. M. Torralba, M. Echeverry*

5. *Organisation of primary-secondary school and bachelor-master students visits to IMDEA Materials, 10 visits along 2021 with over 150 visitors.*

5.7. IMDEA Materials in the media

1. *Madrid inaugura en Getafe un laboratorio de investigación de materiales sanitarios.* Cadena SER
2. *Especial La Ventana de Madrid 8-M desde el IMDEA.* M. T. Pérez-Prado. Cadena SER
3. *Nuevos materiales para prótesis óseas.* J. LLorca. RNE
4. *De la industria aeroespacial a los nanotubos de silicio para baterías: Getafe alumbra el futuro.* J. J. Vilatela. La Razón
5. *Así es el laboratorio de Getafe que busca materiales para regenerar el cuerpo.* ABC
6. *Ciencia 'made in Madrid', élite mundial.* ABC
7. *Floatech apuesta por el silicio para revolucionar la futura industria de las baterías.* J. J. Vilatela. El Español
8. *José Manuel Torralba, director del IMDEA Materiales, primer español en ser premiado con la Medalla de Oro de la FEMS.* J. M. Torralba. Europa Press
9. *Grupo Antolin colabora con Imdea para desarrollar baterías flexibles adaptables al interior del coche.* J. J. Vilatela. Europa Press
10. *La primera spin-off de IMDEA Materiales fabricará electrodos de baterías para vehículos eléctricos.* J. J. Vilatela. Notiweb Madri+d
11. *Six research teams win Carbon Hub funding.* J. J. Vilatela, EurekAlert
12. *La startup smartHAPS y el Instituto IMDEA Materiales se lanzan a la conquista de la estratosfera.* D-Y Wang. Actualidad Aeroespacial
13. *Grupo Antolin está desarrollando baterías flexibles adaptables al interior del coche eléctrico.* J. J. Vilatela. Híbridos y Eléctricos
14. *Implantes inteligentes para cirugías de mínima invasión.* J. M. Molina-Aldareguia. Infosalus
15. *La Comunidad de Madrid instala un nuevo laboratorio de cultivo celular para investigar materiales innovadores de uso sanitario.* Economía de hoy
16. *La Comunidad instala un nuevo laboratorio de cultivo celular para investigar materiales de uso sanitario.* Madrid Actual
17. *La Comunidad de Madrid investigará materiales innovadores para uso sanitario.* MSN Noticias

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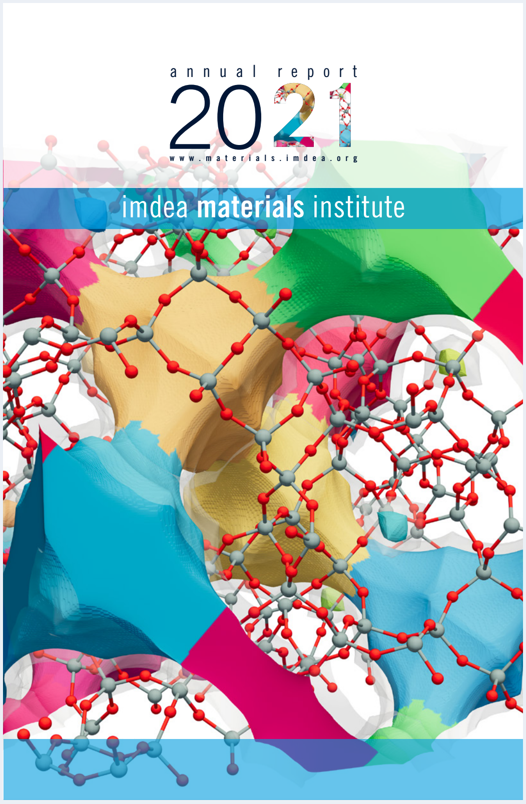

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