institute
IMdea
materials

Encompassing Research of Excellence
and Technology Transfer

EUROPEAN UNION
STRUCTURAL FUNDS

Comunidad
de Madrid

EXCELENCIA
MARÍA
DE MAEZTU

www.materials.imdea.org

Research Projects Offer 2024
2024 年可申请研究项目和方向

1. Topological deformations in mechanical metamaterials
机械超材料的拓扑变形研究

Supervisor: **Dr. Johan Christensen**

2. Peering into the origin of grain refinement and twin boundaries in metallic alloys
金属合金中晶粒细化和孪晶界的起源研究

Supervisor: **Dr. Maria Teresa Perez Prado & Dr. Damien Tourret**

3. Building computational tools for the design of novel sustainable metallic alloys
构建用于设计新型可持续金属合金的计算方法

Supervisors: **Prof. Dr. José M. Torralba** & **Dr. Damien Tourret**

4. Development of autonomous laboratory for discovery and processing of multifunctional nanocomposites
多功能纳米复合材料发现和加工的自动实验室研究

Supervisor: **Dr. Maciej Haranczyk**

5. Development and deployment of intelligent digital twins for manufacturing
用于制造业的智能数字孪生的发展与运用

Supervisor: **Prof. Carlos González**

6. Multi-objective topology optimization of microstructures
微观结构多目标拓扑优化研究

Supervisor: **Prof. Carlos González**

7. Novel biomaterials development for tissue engineering and regenerative medicine
用于组织工程和再生医学的新型生物材料研究

Supervisor**: Dr. Jennifer Patterson**

1. Topological deformations in mechanical metamaterials

机械超材料的拓扑变形研究

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Johan Christensen

Email: : johan.christensen@imdea.org *Tel:* +34 91 549 3422.

Short Bio – Google Scholar – Relevant papers

Project description

High-speed technologies, such as aerospace and vehicle engineering, demand light-weight yet high-performance materials. Architected metamaterials (AMs) consist of periodic arrangements of nodes and struts, requiring less mass that makes them potentially resource- and energy- efficient, thus being an ideal candidate for such engineering applications. Under heavy loads, AMs usually fail from strain localization, i.e., shear bands (SBs). Thus, understanding and controlling SBs is the key to designing high-performance AMs. Efforts so far have focused on understanding and predicting SB formations yet engineering them through topological design constitutes a completely different avenue. Inspired by metallurgical approaches, stiff inclusions, also known as precipitates, have been introduced to AMs at the mesoscale, which serves the purpose to guide and steer the evolution of SBs. Further, precipitates are widely observed in both biological materials and engineering alloys, showing benefits to strength and toughness. Also, engineering SBs based on AMs with consideration of lattice topology and material plasticity will be a competitive driver of modern technology development.

IMDEA Material's acoustic and mechanical metamaterials research group is a world-renowned team, known to have combined contemporary condensed matter physics and engineered acoustic and elastic metamaterials. Through theory, computations, and experiments, their mission is to broaden the understand of basic and applied sound and vibrations. See, for example: Nature 618, 687 (2023).

This project aims at shedding light into elusive aspects of the shear-band-relevant response of AMs with consideration of precipitates and plasticity, focusing on the formation and evolution of shear bands, the effect of lattice topology, the overall mechanical properties such as stress-strain relation and toughness, and the optimized mesoscale structures for industry-level applications. This will be accomplished by creating a theoretical framework combining theoretical modelling, finite element methods (FEM) simulations, and machine learning (ML). Subsequently, the theoretical results will be validated in experiments. To achieve the objectives, it is expected that the candidate has knowledge in continuum mechanics, mechanical instabilities, finite element simulations, and/or condensed matter physics.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA

The candidate will acquire advanced skills in mathematical modelling and experimental studies concerning topological physics and symmetry related mechanical deformations. The results will be presented in high-impact peer-reviewed journals and at international conferences. The Institute also provides a range of training events for "soft" transversal skills and language classes (Spanish, English).

Skills required for CSC student/scholar

A solid background in solid mechanics or condensed matter physics is required. Experience in computational modelling and scientific programming. Fluent English (oral and written) is mandatory.

Remarks

This project can host 1 PhD student.

2. Peering into the origin of grain refinement and twin boundaries in metallic alloys
金属合金中晶粒细化和孪晶界的起源研究

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Maria Teresa Perez Prado, Senior Researcher – Sustainable Metallurgy
Dr. Damien Tourret, Researcher – Modeling & Simulation of Materials Processing

Email: teresa.perez.prado@imdea.org / *damien.tourret@imdea.orgTel:* +34 91 549 3422
Dr. Perez Prado: Short Bio – Google Scholar – LinkedIn – WebsiteDr. Tourret: Short Bio – Google Scholar – LinkedIn – Website

Project description

It was recently shown that dramatic microstructure refinement in metallic alloys may be induced by the nucleation of icosahedral quasicrystal (QC) patterns in the liquid during solidification. Since the first observation of this mechanism in Al alloys, it was identified in several alloys, including in systems with no known quasi-crystalline phases. A challenge in identifying this mechanism is the need for deep crystallographic analysis of grain orientation relations, so far limited to small patches of at most a dozen of grains. The objective of the project is to get a deeper understanding of this QC- mediated grain refinement. In order to identify orientation relationships, crystallographic analysis tools will be developed and applied at a much broader scale than currently possible. The study will involve advanced characterization, in particular electron microscopy and diffraction (EBSD), combined with computational data analysis, including machine learning (ML) exploration of crystallographic data. This research will advance the state-of-the-art in computational- and ML-guided microstructure analysis. It is expected to lead to the discovery of the QC-mediated nucleation mechanism in a broad range of alloys, and possibly the existence of new quasicrystal patterns unidentified to date.

Project outcomes that CSC student/scholar could expected to achieve via workingin IMDEA

The candidate will acquire advanced skills in physical metallurgy, in particular microstructural characterization, a strong expertise in crystallography, and broad knowledge on metallic materials processing (e.g. 3D printing). The fellow will be trained in computational thermodynamics (CalPhaD), scientific programming (Python) for data analysis, and gain hands-on experience in the use of Machine Learning for microstructural analysis. Results will be presented in high-impact peer-reviewed journals and at international conferences. The Institute also provides a range of training events for “soft” transversal skills, as well as language classes (Spanish, English).

Skills required for CSC student/scholar

A background in metallurgy, materials science, materials physics, or a related field is required. Experience and/or strong interest in metallic materials, characterization, and crystallography, and some programming (Python) or Machine Learning knowledge will all be highly valued. Fluent English (oral and written) is mandatory.

Remarks

This project can host 1 PhD student

3. Building computational tools for the design of novel sustainable metallic alloys
构建用于设计新型可持续金属合金的计算方法

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Damien Tourret, Senior Researcher – *Modeling & Simulation of Materials Processing*
Email: damien.tourret@imdea.org Short Bio – Google Scholar – LinkedIn – Website

Prof. Jose Manuel Torralba, Senior Researcher – *Sustainable Powder Technologies*
Email: josemanuel.torralba@imdea.org Short Bio – Google Scholar – LinkedIn – Website

Project description

The research will focus on the development of computational tools for the exploration and design of novel metallic alloys. The methods will combine the use of computational thermodynamics (e.g. CalPhaD method) with machine learning to explore the enormous multicomponent alloy design space, validated by laboratory experiments, characterization, and testing. One central goal is to produce a practical alloy design tool for the use of alloy mixtures to produce new high-entropy alloys – e.g. mixing electronic waste with common "commodity" alloys to produce recycled alloys with competitive properties and performance for structural applications.
The candidate will be jointly appointment in a computational (DT) and an experimental (JMT) group. Hence, while the key focus of the project is computational, several laboratory activities are expected. The fellow will provide simulations in support of several ongoing projects within the host groups. Moreover, the project itself will require a validation of the designed alloys in the laboratory, which will be performed by the fellow, supported by other group members.

Project outcomes that CSC student/scholar could expected to achieve via workingin IMDEA

The candidate will develop computational tools to design the next generation of sustainable alloys. On the computational side, the fellow will acquire knowledge and skills in thermodynamics (e.g. complex multicomponent phase diagrams), scientific programming (mostly Python), and machine learning tools to explore the wide multidimensional alloy space. From the experimental point of view, the fellow will get hands-on experience in metallic material production (e.g. casting), metallurgical analysis (e.g. electron microscopy and diffraction analysis) and mechanical testing (e.g. macro/micro-hardness and tensile testing). The doctoral research is decidedly positioned in the scope of sustainable manufacturing, and expected to lead to several high-impact papers in peer-reviewed journals and presentations at international conferences, and to a high employability in both academic and industrial (e.g. manufacturing, aeronautics, automotive, etc.) sectors.

Skills required for CSC students/scholars

The candidate should have a degree in Materials Science & Engineering, Mechanical and/or Metallurgical Engineering, or a related discipline, with excellent academic credentials. Candidates with knowledge in scientific programming (e.g. Python, C, Fortran), computational thermodynamics (e.g. CalPhaD) or hands-on experience or interest in metallurgy (e.g. casting) and metallography (e.g. microscopy, mechanical testing) are strongly encouraged to apply.
Fluent English (oral and written) is mandatory.

Remarks

The project can host 1 PhD student.

4. Development of autonomous laboratory for discovery and processing of multifunctional nanocomposites

多功能纳米复合材料发现和加工的自动实验室研究

Duration of project and time-length for hosting CSC student/scholar

4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Maciej Haranczyk – Computational and Dara-Driven Materials Discovery
Email: *maciej.haranczyk@imdea.org* *Tel:* +34 91 549 3422
Short Bio – Google Scholar – LinkedIn

Project description

The research will focus on the development of novel nanocomposites incorporating sustainable polymers and advanced functional additives, especially in the context of energy and transport applications. Traditionally, the development is a slow and iterative process of identification of the composition and processing parameters that achieve just right properties required by a given application. In this PhD project, we aim to build an autonomous laboratory, equipped with robots and guided by artificial intelligence to perform the nanocomposite development with little-to-none intervention by a human researcher. Such concept is often referred to as a self-driving laboratory or a material acceleration platform. In this case, we specifically target polymer-based systems, which can be investigated in bulk, as twin films or coatings. In this PhD project will develop both hardware and software solutions to perform the polymer processing and characterization steps automatically. An example of similar on-going work can be viewed in a recent article in Digital Discovery (DOI: 10.1039/D3DD00141E).

Project outcomes that CSC student/scholar could expected to achieve via workingin IMDEA

The candidate will gain experience in the emerging field of laboratory automation, and will develop algorithms and open-source hardware to enable autonomous and/or remote laboratory work related with polymer processing and characterization. The doctoral research is expected to lead to several high-impact papers in peer-reviewed journals and presentations at international conferences.

Skills required for CSC student/scholar

The candidate should have either a) a degree in Materials Science and Engineering or Chemistry with excellent academic credentials and experience in polymer processing, and be interested in learning more about automation, machine learning and data-driven experimentation; or b) a degree in Computer Science, Mechanical Engineering or Robotics, and be interested in applications to material science.

In all cases, candidates with knowledge in simulation of materials, computer vision, machine learning and experience in scientific programming (C, C++, Python) are strongly encouraged to apply. Fluent English (oral and written) is mandatory.

Remarks

This project can host 1 PhD student.

5. Development and deployment of intelligent digital twins for manufacturing
用于制造业的智能数字孪生的发展与运用

Duration of project and time-length for hosting CSC student/scholar
4 years

Name of the project leader/supervisor, and contact info including webpage link
Prof. Carlos González at UPM, Structural Composites Group at IMDEA

Email: c.gonzalez@upm.es, carlosdaniel.gonzalez@imdea.org
Tel: +34 91 549 3422
Short Bio – Google Scholar – LinkedIn

Project description
Rapid advances in new-generation information technologies such as big data analysis, the Internet of Things, edge computing, and artificial intelligence (AI) are pushing traditional manufacturing to intelligent manufacturing within the Industry 4.0 concept. Smart Manufacturing of Polymer Matrix Composites (PMCs), including methods to control the process while guaranteeing the article's final quality, is now under developing development and deployment. The project is aimed at the implementation of digital twins (DT) for the manufacturing of structural composites based on a set of possible techniques, including injection/infusion, 3D printing or hot-compression consolidation. The DT will be based on deep-learning architectures that will analyze the information recorded by sensors (pressure, temperature, cure, etc.) for the on-the-fly prediction of a set of quantities of interest (flow, pressure, temperature evolution) during the process. The project will focus on using the DT for actuating during the process to recover from possible process disturbances. Algorithms for intelligent DT based on the reinforcement learning paradigm will be at the project's core. The candidate will conduct comprehensive research based on advanced virtual processing modelling, artificial intelligence, and physical deployment at the lab-scale floor level.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA
The candidate will acquire advanced skills in composite manufacturing, virtual processing (fluid and solid mechanics), and a strong expertise in machine learning and artificial intelligence. The fellow will be trained in data science (Keras, TensorFlow,…), scientific programming for data analysis, sensoring and actuation for smart manufacturing. Results will be presented in high-impact peer-reviewed journals and at international conferences. The Institute also provides a range of training events for "soft" transversal skills and language classes (Spanish, English).

Skills required for CSC students/scholars
A solid background in fluid/solid mechanics is required. Experience in computational modelling, scientific programming, data-science, and artificial intelligence will be evaluated. Fluent English (oral and written) is mandatory.

Remarks
The project may host 1 PhD student.

6. Multi-objective topology optimization of microstructures
微观结构多目标拓扑优化研究

Duration of project and time-length for hosting CSC student/scholar
4 years

Name of the project leader/supervisor, and contact info including webpage link
Prof. Carlos González at UPM, Structural Composites Group at IMDEA

Email: c.gonzalez@upm.es, carlosdaniel.gonzalez@imdea.org
Tel: +34 91 549 3422
Short Bio – Google Scholar – LinkedIn

Project description
Foams and lattices are widely used for creating lightweight, load-bearing structures. Additionally, these microstructures can be used or added for further functions, such as sound, heat insulation, or shielding. The topology of the microstructure will condition the functionality of the resulting part. Topology optimization is a vibrant area of research which allows to optimize material distribution in a given design space as to maximize performance. Recent work has demonstrated that topology optimized microstructures outperform homogeneous microstructures in terms of structural performance and material use, which adds an additional environmental benefit. Optimization towards vibroacoustic or heat transfer performance is also being explored.
However, optimization for multifunctional objectives remains a challenge, due to the complex multi-physical design requirements as well as the need to balance conflicting specifications. The 3D nature of the parts under design adds further complexity.
The aim of this project is the development of a versatile topology optimization framework for the vibroacoustic and thermal design of sandwich structure cores while constraining volume and structural stiffness.
This research proposes a data-driven approach for generating microstructures, based on a fully convolutional neural network (CNN).
The candidate will conduct comprehensive research on computer vision (CV) tasks, such as image classification/labeling, image segmentation (pixel-wise labeling), and object localization coupled with multi-objective topology optimization algorithms.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA
The candidate will acquire a strong expertise in machine learning and artificial intelligence and advanced skills on additive manufacturing. The fellow will be trained in data science, scientific programming for data analysis, and heat and sound transmission through metamaterials. Results will be presented in high-impact peer-reviewed journals and at international conferences. The Institute also provides a range of training events for “soft” transversal skills and language classes (Spanish, English).

Skills required for CSC students/scholars
A solid background in solid/fluid mechanics is required. Experience in computational modelling, scientific programming, data-science, and artificial intelligence will be evaluated. Fluent English (oral and written) is mandatory.

Remarks
This project can host 1 PhD student.

7. Novel biomaterials development for tissue engineering and regenerative medicine
用于组织工程和再生医学的新型生物材料研究

Duration of project and time-length for hosting CSC student/scholar
4 years

Name of the project leader/supervisor, and contact info including webpage link

Dr. Jennifer Patterson, Researcher,
Head of *Biomaterials and Regenerative Medicine* Group

Email: jennifer.patterson@imdea.org; *Tel:* +34 91 549 3422 ext. 1086
Links: 0000-0001-6927-6548 (ORCID); C-4985-2014 (ResearcherID); 56234220300 (Scopus); https://www.linkedin.com/in/jennifer-patterson-5a93155 (LinkedIn); https://materials.imdea.org/people/jennifer-patterson/ (IMDEA website)

Project description
The research group is centered around the synthesis of novel biomaterials, with a particular focus on hydrogels; the processing of biomaterials into complex 3D structures (scaffolds); the evaluation of physicochemical properties of the materials, such as morphology and mechanical properties; and the characterization of the materials' and scaffolds' cytocompatibility and biological functionality in vitro. The specific project will be developed in line with the interests of the CSC student/scholar but should be related to an ongoing project in the lab, which include:

- BIOMET4D, which seeks to develop load-bearing and shape-morphing implants made of biodegradable metals – the materials characterization of 3D printed biodegradable metal samples and in their characterization for in vitro cytotoxicity
- CARDIOBOOST, which seeks to develop biomaterials-based approaches to promote the differentiation of stem cells into mature cardiomyocytes – the synthesis and characterization of novel polymer-based resins for 3D printing or the evaluation of the growth and alignment of relevant cell types on 3D patterned substrates
- ReCoil3D, which seeks to develop dynamic reinforced extracellular matrix-derived scaffolds with oriented pores for articular cartilage tissue engineering – the mechanical and morphological characterization of the porous scaffolds and the evaluation of chondrogenic differentiation of mesenchymal stem cells cultured within the scaffolds
- Fundamental development of novel hydrogels, based on gelatin, chitosan, or a synthetic low molecular weight gelator, as biomaterials

Project outcomes that CSC student/scholar could expected to achieve via workingin IMDEA
The CSC student/scholar will be introduced and trained to master experimental techniques, including chemical synthesis and analysis (FTIR, GPC, TGA, DSC, etc.), mechanical testing and rheology, additive manufacturing/3D printing, microscopy (SEM, confocal), and cell culture (viability and proliferation as well as biochemical assays). Results will be published in high-impact peer-reviewed journals and presented at top international conferences. IMDEAprovides a broad range of training activities for transversal skills and languages (Spanish, English).

Skills required for CSC students/scholars
A background in materials science, biomedical engineering, chemistry, chemical engineering, or a related field is required. Previous experimental experience in hydrogel chemistry, characterization of the physical and chemical properties of biomaterials, 3D printing, and/or cell culture will be strongly valued. Fluent English (oral and written) is mandatory.

Remarks

This project can host 1 PhD student.