institute IMdea materials

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Research Projects Offer 2023
2023 年可申请研究项目和方向

1. Multiscale modeling of microstructure growth during the solidification of alloys
合金凝固过程中微观结构生长的多尺度建模

Supervisors: **Dr. Damien Tourret**

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. Development of novel high entropy alloys (HEAs) via powder metallurgy (PM) for hydrogen storage applications
通过粉末冶金方法开展用于储氢应用的新型高熵合金研究

Supervisors: **Prof. Dr. José M. Torralba**

4. 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

Supervisors: **Prof. Carlos González**

5. Advanced high strength steels processed via ultrafast heating
通过超快加热方式处理的高强度钢材料的研究

Supervisors: **Dr. Ilchat Sabirov**

6. Physical simulation of joining of dissimilar materials
异形材料连接的物理模拟行为研究

Supervisors: **Dr. Ilchat Sabirov**

7. Mechanism of competitive grain growth during directional solidification of bicrystals
双晶定向凝固过程中竞争晶粒生长机理研究

Supervisor**: Dr. Srdjan Milenkovic & Dr. Damien Tourret**

8. High-performance biobased polymers for advanced applications
高性能生物基聚合物材料及其先进应用

Supervisor**: Prof. Dr. De-Yi Wang**

1. Multiscale modeling of microstructure growth during the solidification of alloys
合金凝固过程中微观结构生长的多尺度建模

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, Researcher – Modeling & Simulation of Materials Processing
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Short Bio – Google Scholar – LinkedIn – Website

Project description

The research will focus on multiscale modeling of dendritic microstructure growth during the solidification of alloys (such as in casting, welding, or additive manufacturing processes). These microstructures and their morphologies strongly affect the thermomechanical properties of technological components. Hence, they occupy a central role in developing innovative alloys and processing routes for next generations of high-performance structural materials. Specifically, the project will explore the effect of fluid flow on the selection of dendritic microstructures. One objective is to extend a recently-developed unique multiscale approach (*Acta Materialia 234 (2022) 118035. https://doi.org/10.1016/j.actamat.2022.118035*) to include the motion of solid crystals, in order to explore and elucidate the effect of stray grain buoyant motion (e.g. settling or floating) during solidification (*Advanced Engineering Materials 17 (2015) 454-459. https://doi.org/10.1002/adem.201400469*). While the PhD project is mostly focused on modeling, internal and international collaborators will provide experimental measurements that will be crucial to the validation of the developed model. The model will, in turn, be used to simulate and provide original interpretations to experimental observations and measurements.

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

The candidate will develop computational codes to model dendritic crystal growth, based on a newly introduced multiscale modeling approach. The candidate will acquire knowledge and skills in thermodynamics and kinetics of phase transformations, computational fluid dynamics, fluid-particle interactions, and high-performance parallel computing. Research activities will also explore coupling pathways with models applicable at other length and time scales, such as phase-field, molecular dynamics, and macroscopic continuum thermomechanics. 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 a degree in Materials Science and Engineering, Materials Physics, Mechanical Engineering, or a related discipline, with excellent academic credentials. Candidates with knowledge in numerical simulation of materials (e.g. fluid dynamics, thermomechanics, thermodynamics, etc.) and experience or interest in scientific programming (C, C++) are strongly encouraged to apply. 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

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Dr. Perez Prado: Short Bio – Google Scholar – LinkedIn – Website Dr. 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. Development of novel high entropy alloys (HEAs) via powder metallurgy (PM) for hydrogen storage applications
通过粉末冶金方法开展用于储氢应用的新型高熵合金研究

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

3-4 years

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

Prof. Dr. José M. Torralba
Head of the Powder Metallurgy Group

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Project description

Hydrogen is a valid clean fuel, during its combustion, this element does not generate harmful gas emissions associated with fossil fuel combustion. To ensure a proper hydrogen storage, new alloys must be developed with a high resistance to hydrogen embrittlement (HE), which can cause mechanical failure in high strength alloys. Recently, a new class of alloys, the high-entropy alloys (HEAs), have been investigated for their hydrogen storage properties. In a HEA, five or more elements are mixed in approximately equimolar ratios. HEAs with a FCC-type structure have a large capacity to store hydrogen, also they demonstrate excellent H/M ratios (>2) and hydrogenate reversibly near ambient conditions, combined, these properties indicate the utility of these alloys in versatile hydrogen storage applications. In this project, the development of new high entropy alloys (HEAs) by powder metallurgy (PM) is proposed. Starting with the selection of the adequate alloy compositions, these will be processed from the starting powders to consolidation and posterior heat treatments. After this, the tolerance of the HEAs to HE will be studied regarding the possible alterations in the mechanical and microstructural features.

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

The student will be introduced to the use of different powder metallurgy processes, like consolidation techniques such as field assisted sintering (FAS), spark plasma sintering (SPS) or selective laser melting (SLM). Moreover, microstructural characterization techniques like SEM, TEM, EBSD will be employed; also, mechanical testing will be developed such as hardness measurements, microtensile, or compression tests. The results of the investigation will be published in high impact international peer-reviewed journals and conferences. In the case of collaborations with other scientific institutions, if necessary, the student may carry out research stays during which specific characterization tests will be performed.

Skills required for CSC students/scholars

A solid background in physical metallurgy/materials science is required. Experience in computational thermodynamics will be valued. Basic knowledge of phase diagrams, metallography, powder metallurgy and mechanical behaviour of metallic materials. Fluent English (oral and written) is mandatory. Experience in writing scientific papers will be valued.

Remarks

The project can host 1 PhD student.

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4. 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

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Tel: +34 91 549 3422
Prof. Perez Prado: 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 workingin 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 student/scholar
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
This project can host 1 PhD student.

5. Advanced high strength steels processed via ultrafast heating

通过超快加热方式处理的高强度钢材料的研究

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. Ilchat Sabirov, Senior Researcher
Head of Physical Simulation Group

Email: *ilchat.sabirov@imdea.org*
Tel: +34 91 549 3422
Link to ShortBio - www.materials.imdea.org

Project description

This project will focus on development of ultrafast heating (UFH) for fabrication of advanced high strength steels. The UFH process is a valuable alternative to other industrially used thermal treatment cycles, since it provides a range of advantages including grain refinement and formation of multiphase microstructures in low alloyed steels, which result in improved mechanical strength and ductility. Moreover, UFH process is very short compared to the conventional thermal treatments performed in continuous annealing lines, that results in significant productivity gains and lower price of the product. The main outcome of the project will be fundamental understanding of the effect of UFH process and steel chemistry on the microstructure and properties of steels and mechanisms underlying microstructure evolution during UFH process.

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

The CSC student will gain a deep fundamental knowledge in the area of thermo-mechanical processing and characterization of advanced high strength steels. The student will develop skills in physical simulation using thermo-mechanical simulator GLEEBLE, advanced microstructural characterization techniques, such as SEM, FIB, TEM and EBSD, and mechanical testing, including fatigue testing and in situ testing inside the SEM. The student will work in a very close collaboration with leading researchers from European partner universities. An opportunity for obtaining European PhD degree can also be offered.

Skills required for CSC students/scholars

Background in Materials Science and Engineering/Physics/Metallurgy and expertise in microstructural characterization and/or mechanical behavior of metallic materials is desirable. Excellent academic credentials as well as fluent spoken and written English are necessary.

Remarks

The project may host 1 PhD student.

6. Physical simulation of joining of dissimilar materials
异形材料连接的物理模拟行为研究

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. Ilchat Sabirov, Senior Researcher
Head of Physical Simulation Group

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Project description
Emerging trends in manufacturing such as light weighting, increased performance and functionality increases the use of multi-material, hybrid structures and thus the need for joining of dissimilar materials. The properties of the different materials are jointly utilised to achieve product performance. The joining processes can, on the other hand be challenging due to the different properties of the joined materials. Development of processing routes for joining of dissimilar materials is always a very challenging task which is typically based on the trial and error approach that requires significant resources. Physical simulation of metallurgical processes can dramatically reduce time and cost of development of processing routes. This project will focus on development of a novel physical simulation tool for prediction of weld quality, microstructure and properties of dissimilar materials (steels and Al alloys) joined by friction melt bonding (FMB), which is a novel joining technique. The main outcomes of this project will be a new tool for physical simulation of joining of dissimilar materials and fundamental understanding of the effect of FMB parameters on the weld quality, microstructure and properties of bonding layer.

Project outcomes that CSC student/scholar could expected to achieve via working in IMDEA
The CSC student will gain a deep fundamental knowledge in the area of joining of metallic materials. The student will develop skills in physical simulation of joining processes using thermo-mechanical simulator GLEEBLE, advanced microstructural characterization techniques, such as SEM, FIB, TEM and EBSD, and mechanical testing, including in situ testing in SEM chamber and nanoindentation. The student will work in a very close collaboration with leading researchers from the Université Catholique de Louvain (Belgium). An opportunity for obtaining European PhD degree and a stay with the Université Catholique de Louvain can also be offered.

Skills required for CSC students/scholars
Background in Materials Science and Engineering/Physics/Metallurgy and expertise in microstructural characterization and/or mechanical behavior of metallic materials is desirable. Excellent academic credentials as well as fluent spoken and written English are necessary.

7. Mechanism of competitive grain growth during directional solidification of bicrystals
双晶定向凝固过程中竞争晶粒生长机理研究

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. Srdjan Milenkovic, Senior Researcher,
Head of *Solidification Processing and Engineering* GroupDr. Damien Tourret, Researcher
Head of *Modeling & Simulation of Materials Processing* Group

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Project description
Directional solidification is a well-established industrial process. It is the main manufacturing route for single crystals superalloys used in high-temperature applications, e.g. aeroengine turbine blades. Yet, casting a single crystal remains challenging due to the common occurrence of defects and low angle boundaries. The aim of this project is to systematic investigate the formation of stray grains and grain boundaries during polycrystalline dendritic growth, since competitive growth plays a key role in the single crystal quality. Methods will combine both experiments and modelling. The experimental part will include directional solidification in a Bridgman furnace using spiral selector or seed crystals to produce controlled bicrystal samples. The modelling tasks will rely on quantitative 3D phase-field modeling. This will be among the first in-depth studies of dendritic growth competition in three-dimensional samples under realistic casting conditions.

Project outcomes that CSC student/scholar could expected to achieve via workingin IMDEA
During the project the student will be introduced and trained to master several experimental (directional solidification, metallographic and microstructure analysis using optical, scanning and transmission electron microscopy, EBSD) and modelling techniques (process-scale thermal analysis, microstructure-scale phase-field method, computational thermodynamics (CalPhaD)). Results will be published in high-impact peer-reviewed journals and presented at top-level international conference. The Institute also provides a broad range of training events for "soft" or transversal skills, as well as languages (Spanish, English).

Skills required for CSC students/scholars
A background in metallurgy (phase diagrams, metallography, casting), materials science, or a related field is required. Previous experience in experimental metallurgy and/or scientific programming will be strongly valued. Fluent English (oral and written)is mandatory.

Remarks
This project can host 1 PhD student.

8. High-performance biobased polymers for advanced applications
高性能生物基聚合物材料及其先进应用

Duration of project and time-length for hosting CSC student

4 years

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

Prof.Dr. De-Yi Wang, FRSC, Senior Researcher
Head of the High Performance Polymer Nanocomposites (HPPN) Group

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Link to ShortBio
http://www.materials.imdea.org/groups/hppn/

Project description

This project would focus on the development of new generation bio-based polymers for advanced applications, such as using as adhesive, bio-resins, etc., via multidisciplinary approach. The ground-breaking idea would be a combination of innovative molecular design, chemistry synthesis and functionalization. Advanced experimental analytical techniques will be employed to understand structure-property relationship. This is a unique opportunity for an enthusiastic young scientist to join an excellent international lab located at an excellent research environment with all the start-of-the-art core facilities.

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

During the project, student will learn the knowledge on design of the functional polymers and development of high-performance bio-based polymers and will be trained in advanced characterization techniques applied to new multifunctional nanomaterials. The results of the investigation will be expected to be published on high impact international journals. The student would be working in a really international environment and performing research at a high international standard and in the frontier of material science and technology.

Skills required for CSC student/scholar

Solid knowledges in polymer chemistry or functional polymers; good spoken and written English; excellent team cooperation personality

Remarks

The project will host 1 PhD student. High Performance Polymer Nanocomposites (HPPN) Group in IMDEA Materials Institute has set up close collaboration with some top-level research institution, such as ETH (Swiss Federal Institute of Technology in Zürich, Switzerland), IPF (Leibniz Institute of Polymer Research Dresden, Germany), etc. Consequently, the student will be involved in an environment with many potentialities and the perfect expertise for the fulfillment of the project.