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**Research Projects Offer 2022**  
**2022 年可申请研究项目和方向**

**1. 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**

**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 Tournet**

**3. Breakthrough application of W free Co based superalloys via advanced sustainable manufacturing technologies**  
通过先进可持续制造技术实现无 W 钴基高温合金的创新性研究

Supervisor: **Prof. Dr. José M. Torralba & Dr. Ahad Mohammadzadeh**

**4. 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 Tournet**

## **1. 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

Email: [josemanuel.torralba@imdea.org](mailto:josemanuel.torralba@imdea.org)

Tel: +34 91 549 3422

[Link to ShortBio](#)

<http://www.materials.imdea.org/>

### **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 working in 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.

## **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](mailto:teresa.perez.prado@imdea.org) / [damien.tourret@imdea.org](mailto:damien.tourret@imdea.org)

*Tel:* +34 91 549 3422

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 working in 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. Breakthrough application of W free Co based superalloys via advanced sustainable manufacturing technologies**

通过先进可持续制造技术实现无 W 钴基高温合金的创新性研究

#### **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. Jose Manuel Torralba, Scientific Director

Dr. Ahad Mohammadzadeh, Post-doctoral Research Associate

Powder Metallurgy Group

Email: [josemanuel.torralba@imdea.org](mailto:josemanuel.torralba@imdea.org) and [ahad.mohammadzadeh@imdea.org](mailto:ahad.mohammadzadeh@imdea.org)

Tel: +34 91 549 3422

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#### **Project description**

Over the recent decades, the high-temperature capability of Ni-based superalloys has been limited since the gamma prime ( $\gamma'$ ) solvus temperature gets closer to the Ni melting point. Therefore, their maximum operative temperature is a growing concern towards the sustainable development of advanced jet engines and gas turbine applications. Co based superalloys strengthened by coherent L12 ordered  $\gamma'$  precipitate are promising alternatives for overcoming Ni-based superalloys obstacles. However, the emergence of novel Co based superalloys requires the use of modern sustainable manufacturing technologies (e.g. powder technology, powder metallurgy, and additive manufacturing) to produce high tech, end-use, cost-effective, and eco-friendly products. This proposal aims to develop novel W free Co based superalloys with low density and high specific yield strength using a sustainable metallurgy framework for high-temperature applications. For this aim, after optimizing the chemical composition of the proposed alloys, they will be gas-atomized to produce the required powders for advanced manufacturing techniques, such as field-assisted sintering (allowing full density materials) and selective laser melting (allowing full density and complex shapes). Finally, the developed materials will be post-processed to optimize the morphology, distribution, and volume fraction of  $\gamma'$  precipitates. It is worth noting that in all steps, detailed microstructural characterizations and mechanical tests will be conducted to evaluate the high-temperature behavior of the samples.

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

By implementing the project, the student will be trained to advanced manufacturing processes for superalloys (field-assisted sintering and selective laser melting) and also advanced microstructural characterization techniques (e.g. TEM, FEG-SEM, EBSD) and mechanical tests. The results of the investigation will be published in high impact international peer-reviewed journals and conferences. The development of this family of Co base alloys is expected to lead to scientific advances in production of powder for powder metallurgy routes and feedstock for additive manufacturing technologies, and developing engines for the aeronautical industry.

**Skills required for CSC student/scholar**

A solid background in physical metallurgy is required. Experience in computational thermodynamics and additive manufacturing 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**

This project can host 1 PhD student.



#### **4. 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* Group

Dr. Damien Tourret, Researcher  
Head of *Modeling & Simulation of Materials Processing* Group

Email: [srdjan.milenkovic@imdea.org](mailto:srdjan.milenkovic@imdea.org) , [damien.tourret@imdea.org](mailto:damien.tourret@imdea.org)

Tel: +34 91 549 3422

Short Bio: [S. Milenkovic](#), [D. Tourret](#)  
[www.materials.imdea.org](http://www.materials.imdea.org)

#### **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 working in 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.