

## Position Description

### 1. General Information

<b>Name of the position</b>	<b>Optimization of microstructure and mechanical properties of high entropy alloys</b>
<b>Foreseen date of enrolment</b>	1 October 2024
<b>Position is funded by</b>	<ul style="list-style-type: none"> <li>• COFUND, Marie Skłodowska-Curie Actions (MSCA), Horizon Europe, European Union</li> <li>• Institut National des Sciences Appliquées de Lyon (INSA-L)</li> <li>• Deakin University</li> </ul>
<b>Research Host</b>	Institut National des Sciences Appliquées de Lyon
<b>PhD awarding institutions</b>	Institut National des Sciences Appliquées de Lyon & Deakin University
<b>Locations</b>	Primary: Campus de la Doua, Villeurbanne, France Secondary: Geelong, Australia
<b>Supervisors</b>	Prof. Michel Perez (MATEIS Lab, INSA-L) and Prof. Matthew Barnett (Institute for Frontiers Materials, Deakin)
<b>Group of discipline</b>	Metallurgy, mechanics of Materials

### 2. Research topics (only one of these projects will be funded)

#### Project 1: *Significance of model approximations for yield strength predictions of high entropy FCC alloys*

High entropy alloys (HEAs) are an exciting relatively new concept in metallurgy: multiple chemical elements at high concentrations are mixed, leading sometimes to single phase crystalline materials. Several single-phase FCC HEAs have shown impressive yield strength, due to solute strengthening, and the vast composition range of this class of materials opens many possibilities for the design of alloys with superior mechanical properties. Since their discovery, important theories have emerged to predict the composition, strain-rate and temperature dependence of their yield strength. Key ingredients to such models are dislocation/solute interactions, dislocation properties and dislocation line tension, and can be obtained either from empirical potential calculations, ab initio calculations, or from experimental data, depending on the levels of simplifications of the theories (mean/full field approach, elastic theory approximations, sum rules, etc.). How these approximations impact predictions remains elusive, which can be a problem for alloy design. This PhD project will aim at quantifying the consequences of model inadequacies in identifying interesting alloy compositions, and then propose new methodologies for accurate predictions of FCC HEAs yield strength.



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**Supervisors:** Prof. Michel Perez (INSA-L), Prof. Matthew Barnett (Deakin), Prof. Damien Fabrègue (INSA-L) and Dr. Céline Varvenne

**Research Fields:** Applied Science, alloy design, metallurgy, strengthening modeling

### Project 2: *Atomistic comprehensive insights on the dislocation properties of refractory BCC High Entropy Alloys*

Within the active field of High Entropy Alloys (HEAs), the refractory subclasses of alloys are complex substitutional solid solutions made of nearly equal proportions of up to 5-6 refractory elements and have a BCC structure. They have received considerable attention due to their potential for high temperature applications: they exhibit a very high yield strength up to elevated temperatures – thus competing/superseding Ni-based superalloys, and some of them also have a significant ductility at room temperature. However, there is a lack of fundamental knowledge of the dislocation properties in RHEAs, and as a function of alloy composition, even though such properties dictate the exact nature of the mechanisms responsible for the plasticity in these complex materials. The PhD student will develop ad hoc interatomic potentials to systematically investigate the links between composition, dislocation/solute properties, and plasticity mechanisms at the atomic scale. Once these links are established, the student will be able to identify the relevant physical assumptions to be used in the development of mesoscale models of RHEAs yield strength (currently a highly controversial topic in the literature). This will also help to provide guidance for alloy design of RHEAs.

**Supervisors:** Prof. Michel Perez (INSA-L), Prof. Matthew Barnett (Deakin), Prof. Damien Fabrègue (INSA-L) and Dr. Céline Varvenne

**Research Fields:** Applied Science, Engineering, metallurgy, high temperature applications, atomic scale, plasticity

### Project 3: *On the use of precipitation to strengthen High Entropy alloys*

High entropy alloys are an exciting relatively new concept in alloy design. Rather than taking one element and adding small amounts of others to it, high entropy alloys comprise nearly equal parts of up to five or so elements. Interest in this field was initially focused on single phase solid solution materials. More recently, however, the use of hardening precipitation – such as the one in steels or other convention alloys – has been considered to achieve better mechanical strength, leading for example to the so-called high entropy superalloys, that involve complex ordered/disordered phases. This PhD will explore such a strengthening route by adding some specific alloying elements in small quantities to model medium entropy alloys, and by carrying out some heat treatments to involve the precipitation. The newly formed phases will be characterized in detail and their influence on the mechanical properties will be measured. The modeling of the precipitation kinetics will also be performed by physically-based models.

SIMPLIFYING APPROACH : working on MEAs to better elucidate the role of chemistry.

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**Research Fields:** Applied Science, Engineering, metallurgy



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### 3. Employment Benefits and Conditions

INSA Lyon offers a 36-months full-time work contract (with the option to extend up to a maximum of 42 months) with 2 months of probation period and 35 working hours per week.

The remuneration, in line with the European Commission rules for Marie Skłodowska-Curie grant holders, will consist of a gross annual salary of 28,800 EUR. Of this amount, the estimated net salary to be perceived by the Researcher is 1,928 EUR per month. However, the definite amount to be received by the Researcher is subject to national tax legislation.

#### Benefits include

- Becoming a Marie Skłodowska-Curie fellow and be invited to join the Marie Curie Alumni Association.
- Access to the facilities and premises of the two laboratories involved in the project.
- Tuition fees exemption at both PhD awarding institutions.
- Yearly travel allowance to cover flights and accommodation for participating in AUFRANDE events.
- 10,000 EUR allowance to cover flights and living expenses for 12 months in Australia (which may be taken in several blocks over the period of the employment term as best suits the needs of the researcher).
- 25 days paid holiday leave.
- 112 days maternity leave (if applicable).
- 28 days paternity leave (if applicable).

### 4. PhD enrolment

Successful candidates for this position will be enrolled by the following institutions and must comply with their specific entry requirements, in addition to AUFRANDE's conditions.

Applicants must hold a national Master's degree (research) or another qualification conferring the status of Master (5 years of higher education) in a related area.

Applicants should also meet the English Language Entrance requirement of IELTS 6.5 with no band below 6 (for entrance into an Engineering Degree).

#### More information on INSA Lyon's requirements

Visit the website: <https://www.insa-lyon.fr/en/formation-doctorale>



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## More information on Deakin University

Visit the website: <https://www.deakin.edu.au/research/research-degrees-and-PhD/research-applications>



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