# PhD position

## Context and goals of the PhD

### New insights in the reduced mobility description for the modeling of grain growth and recrystallization at the polycrystalline scale

One of the European Union's objectives in climate change consists of reaching net-zero greenhouse gas emissions by 2050. Such perspective puts the metallic materials industry, as a large contributor to carbon emissions, under tremendous pressure for change and requires the existence of robust computational materials strategies to enhance and design, with a very high confidence degree, new metallic materials technologies with a limited environmental impact. From a more general perspective, the in-use properties and durability of metallic materials are strongly related to their microstructures, which are themselves inherited from the thermo-mechanical treatments.

Hence, understanding and predicting microstructure evolutions are nowadays a key to the competitiveness of industrial companies, with direct economic and societal benefits in all major economic sectors (aerospace, nuclear, renewable energy, naval, defence, and automotive industry).

Multiscale materials modeling, and more precisely simulations at the mesoscopic scale, constitute the most promising numerical framework for the next decades of industrial simulations as it compromises between the versatility and robustness of physically-based models, computation times, and accuracy. The DIGIMU consortium and the RealIMotion ANR Industrial Chair are dedicated to this topic at the service of major industrial companies.

In this context, the efficient and robust modeling of evolving interfaces like grain boundary networks is an active research topic, and numerous numerical frameworks exist [1]. In the context of hot metal forming and when large deformation of the calculation domain and the subsequent migration of grain boundary interfaces are involved, only few approaches remain efficient [2,3].

Moreover, the discussion of the classical kinetic equations used at the mesoscopic scale to describe the relation between the driving pressures acting on the grain boundaries and their resulting motion is more and more discussed [4,5]. This PhD will be dedicated to the enrichment of existing full-field front-capturing [6] and front-tracking [7] methods to integrate some new capabilities such as the use of a tensorial reduced mobility description, a better integration of torque terms in 2D and 3D and a disconnection-based description of the involved mechanisms. The developments will be validated thanks to pre-existing experimental and numerical data concerning the evolution of grain boundary interfaces during recrystallization and related phenomena for different materials. They will also be integrated in the DIGIMU® software.


*[1]A. Rollett, G. S. Rohrer, and J. Humphreys, Recrystallization and Related Annealing Phenomena. 3rd Edition, 2017.*

*[2]L. Maire et al. Modeling of dynamic and post-dynamic recrystallization by coupling a full field approach to phenomenological laws. Materials & Design, 133:498–519, 2017.*

*[3]S. Florez et al. A new front-tracking lagrangian model for the modeling of dynamic and post-dynamic recrystallization. Modelling and Simulation in Materials Science and Engineering, 29(3):035004, 2021.*



MINES Paris
CEMEF rue Claude Daunesse CS 10207 06904
Sophia Antipolis, France
marc.bernacki@minesparis.psl.eu
+33 (0)4 93 67 89 23


## Partners

## Keywords

Digital twins - HPC - Computational Metallurgy - Interface networks - Mobility description - Front capturing/tracking algorithms

## Candidate profile and skills

Degree: MSc or MTech in Metallurgy or Applied Mathematics. Skills: Numerical Modeling, Metallurgy, programming, proficiency in English, ability to work within a multi-disciplinary team.

## Offer

The 3-year PhD will take place in CEMEF, an internationally-recognized research laboratory of MINES ParisTech located in Sophia-Antipolis, on the French Riviera. It offers a dynamic research environment, exhaustive training opportunities and a strong link with the industry. Annual gross salary: about 27.7k€. She/He will join the Metallurgy $\mu$Structure Rheology (MSR) research teams under the supervision of Prof. M. Bernacki.


*[4] A. Bhattacharya et al., Grain boundary velocity and curvature are not correlated in ni polycrystals. Science 374, 6564:189–193, 2021.*

*[5] S. Florez et al. Statistical behaviour of interfaces subjected to curvature flow and torque effects applied to microstructural evolutions. Acta Materialia, 222:117459, 2022.*

*[6] B. Murgas et al. Comparative study and limits of different level-set formulations for the modeling of anisotropic grain growth. Materials, 14(14), 2021.*

*[7] S. Florez et al. A 2D front-tracking lagrangian model for the modeling of anisotropic grain growth. Materials, 15(14), 2021.*