

# PhD position

## CONTEXT AND GOALS OF THE PhD

FULL-FIELD MODELING OF SOLID-SOLID PHASE TRANSFORMATIONS, RECRYSTALLIZATION AND GRAIN GROWTH- APPLICATION TO DIFFERENT ALLOYS

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, the RealMotion ANR Industrial Chair and the DIGIMU software package developed by TRANSVALOR S.A. are dedicated to this topic at the service of major industrial companies like Aperam, ArcelorMittal, Aubert&Duval, Constellium, Framatome and Safran.

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. 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, a new promising, in terms of computational cost, 2D front tracking method called ToRealMotion algorithms [1] was recently developed.

This PhD will be firstly dedicated to the extension of existing numerical framework dedicated to the modeling of solid state phase transformations where grain boundaries and subsequent driving pressures are taken into account. Pre-existing developments [2,3] in context of a level-set full-field formulation will be improved and this mechanism will also be integrated to the ToRealMotion front-tracking algorithms [1]. Ostwald ripening, adequate driving pressure leading to complex second phase particle shapes and interaction mechanisms between evolving second phase particles and grain interfaces will also be investigated.

The developments will be tested/optimized thanks to experimental data concerning different alloys

The developments will be integrated in the DIGIMU® software.

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## KEYWORDS

Digital twins - HPC - Computational Metallurgy - Interface networks - Front tracking and front capturing approaches - Solid-state phase transformation.

## CANDIDATE PROFILE AND SKILLS

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

## OFFER

The 3-year Cifre PhD will take place in CEMEF, an internationally-recognized research laboratory of MINES ParisTech in collaboration with Dr. P. De Micheli from the TRANSVALOR company. The PhD student will be located in Sophia-Antipolis, on the French Riviera. She/He will join the Metallurgy  $\mu$ Structure Rheology (MSR) CEMEF research team under the supervision of Prof. M. Bernacki, Dr. M. Bignon, Dr. O. Senninger. Annual gross salary: about 29.4k€ plus additional benefits from TRANSVALOR S.A.

[1] S. Florez, K. Alvarado, D. Pino Muñoz and M. Bernacki. *Computer Methods in Applied Mechanics and Engineering*, 367:113107, 2020.

[2] N. Chandrappa, M. Bernacki, *CSMA 2022*, <https://hal.archives-ouvertes.fr/hal-03717571>

[3] N. Chandrappa, M. Bernacki, *A level-set formulation to simulate diffusive solid/solid phase transformation in polycrystalline metallic materials - Application to austenite decomposition in steels*, *Computational Materials Science*, 216, 2023, <https://doi.org/10.1016/j.commatsci.2022.111840>.