PhD position

Context and goals of the PhD

New 3D Finite-Element Level-Set framework for the modeling of solid-solid phase transformations and grain interfaces for large-scale polycrystals

DIGIMU is an ANR industrial Chair handled by ARMINES MINES ParisTech and co-funded by ANR and an industrial consortium formed by ArcelorMittal, AREVA, ASCOMETAL, AUBERT & DUVAL, CEA and SAFRAN. This Chair deals with the **D**evelopment of an **I**nnovative and **G**lobal framework for the Model**I**ng of **M**icrostr**U**ctural evolutions involved in metal forming processes. DIGIMU® is also the name of the resulting software developed by the company TRANSVALOR as a project partner.

Countless products involved in our every-day life rely on vital metal parts. Optimizing these parts requires a knowledge of how material properties change during forming operations. Although the understanding of the underlying metallurgical phenomena has improved thanks to the continuous progress of experimental facilities, the interest for increasingly fine and predictive simulations has been recently growing. In this emerging context of "digital metallurgy", the DIGIMU Chair and consortium have two main objectives. The first one is to develop an efficient multiscale numerical framework specifically designed to tackle such problems. The second one is to bring the corresponding numerical methods to an industrial level of maturity, by decreasing significantly their computational cost and by validating them against the industrial expertise existing in the DIGIMU consortium.

In order to accurately describe the 3D evolution of polycrystals (recrystallization, phase transformations…), full-field methods such as the phase-field (PF) or the level-set (LS) methods have to be employed. In this context, a new FE numerical framework to model grain growth (GG) and recrystallization (ReX) based on a LS description of the interfaces and meshing/remeshing capabilities has been recently developed[a]. Nowadays, the LS approach is used for Rex/GG modeling in the context of uniform grids with a finite-difference formulation or in a FE framework on unstructured mesh. LS method is also particularly interesting for the modeling of Smith-Zener pinning or promising to deal with high anisotropy level of grain interface properties.

Interestingly, if the LS approach was recently extended to other self-diffusion mechanisms such as spheroidization in titanium alloys or sintering in powder metallurgy, solid-solid phase transformations (SSPT) was not yet adressed despite the obvious interest to couple phases and grains evolutions in the same LS numerical framework. In the proposed PhD project, the existing LS framework will be extended in order to model SSPT. The new proposed formalism will be investigated in context of austenite-ferrite transformations for a steel and evolution of second phase particles for a nickel based superalloys. Moreover it will be compared to pre-existing PF strategy dedicated to this topic.

Finally, the resulting developments will be prepared for integration in the DIGIMU® software package.

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[a]B. Scholtes et al. Computational Materials Science, 2015 109:388-398, and 2016 122:57-71.

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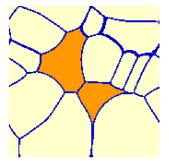☎ +33 (0)4 93 67 89 23

Partners

Keywords

Metallurgy – Solid-solid phase transformations – Grain interfaces – FE Method – HPC – C++.

Candidate profile and skills

Degree: MSc or MTech in Metallurgy, Materials Science or Applied Mathematics, with excellent academic record. Skills: Finite Element Method, Metallurgy, proficiency in English, ability to work within a multi-disciplinary team.

Offer

The 3-year PhD will take place in CEMEF, an internationally-recognised 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: around 26k€. She/He will join the MultiScale Modeling (MSM) and the Metallurgy Structure Rheology (MSR) research teams under the supervision of M. Bernacki, N. Bozzolo and C. Moussa.

Example of phase-field modeling of an austenite-to-ferrite transformation, 2D cut of a 3D simulation - (white) Ferrite grains - (orange) Austenite grains[b]

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[b]M. Militzer, M.G. Mecozzi, J. Sietsma, S. van der Zwaag, 3D phase field modelling of the austenite-to-ferrite transformation. Acta Mater 2006, 54, 3961-3972.