Context and goals of the PhD

Towards an efficient crystal plasticity framework in context of dynamic recrystallization

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

The integration of a crystal plasticity framework into DIGIMU® software is a necessary step toward a more predictive and physically consistent description of polycrystalline material behaviour. Indeed, the mechanical response of some materials depends on complex microstructural features, including grain morphology, crystallographic orientations, local anisotropy, and grain-scale interactions, which cannot be always finely captured by the homogenized approaches currently used in DIGIMU®, whether in the level-set full-field framework [1–3] or in the front-tracking approach developed during the RealIMotion Chair [4]. Through a Material Point Crystal Plasticity framework (MPCP), we have already shown that our grain boundary migration models can be coupled with CPFEM-type formulations for the modeling of discontinuous dynamic recrystallization mechanism [5], but at computational costs too high for industrial simulations or for generating ML training databases. This need is particularly critical for alloys that do not recrystallize discontinuously, where microstructural evolution is driven by gradual and spatially heterogeneous mechanisms such as recovery, subgrain rotation, and continuous recrystallization. For DIGIMU® software, this represents a major scientific challenge. The aim of this PhD is therefore to develop a FFT-based approach [6], suitable for large deformations [7], for our MPCP crystal plasticity module. This approach should support our physical models of both discontinuous and continuous recrystallization. Particular effort will focus on reducing computation times, especially through FFT parallelization. The module will be designed for coupling with DIGIMU® in advanced simulations, while also facilitating the creation of large high-fidelity simulation databases for training machine-learning models.

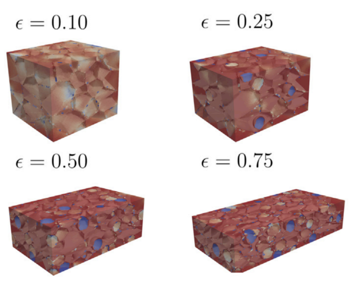

Figure 1: *Dynamic recrystallization modeling within a CPFEM framework* [5].

Experimental datasets on four grades have already been prepared (304L steel, Inconel 718 nickel-based superalloy, AA2139 aluminium alloy, and a Zr–Nb alloy) to test the developed models in line with the consortium's industrial needs.

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Partners

Keywords

Digital twins - HPC - Computational Metallurgy - Dynamic Recrystallization - Front tracking and front capturing approaches - Crystal Plasticity.

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 PhD will take place at CEMEF, an internationally renowned laboratory of Mines Paris PSL. Founded more than 50 years ago, CEMEF conducts cutting-edge research in mechanics, materials, numerical simulation, and artificial intelligence, in close connection with industry and academia. The center brings together around 170 people, including 75 PhD students, in a cosmopolitan and multidisciplinary environment. The PhD candidate will join the research group Metallurgy, μStructure and Rheology (MSR) under the supervision of Marc Bernacki and Daniel Pino Muñoz. The salary is approximately €29k gross per year (before income tax), with benefits including health insurance and meal vouchers.

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