

CONTEXT AND GOALS OF THE PHD

AI FOR ABNORMAL AND CRITICAL GRAIN GROWTH PHENOMENA DISCREMINATION AND AVOIDANCE - APPLICATION TO NICKEL BASE SUPERALLOYS

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. In this context, breakthrough numerical front-capturing and front-tracking strategies to model, at the mesoscopic scale, microstructure evolutions of metallic materials all along complex industrial thermomechanical (TM) processing routes have been developed in CEMEF [1,2].

Abnormal grain growth (AGG) and critical grain growth (CGG) are two well-known metallurgical mechanisms leading to overgrown grains in microstructures without or with stored energy, respectively. As such large grains can be detrimental to the fatigue resistance, it is a critical issue for numerous industrial applications. The understanding and full-field modeling of these mechanisms has greatly been improved in the last decade. A statement at the basis of this proposal is that the partners already have the capability of modeling in full-field context the main mechanisms that can lead to AGG or CGG during annealing [2].

However, from the industrial perspective, the complexity remains that it is generally impossible by looking the final experimental micrograph of the microstructure to discriminate easily and confidently the elements involved in the occurrence of these phenomena and their chronology. This aspect explains one of the current difficulty of optimizing the obtained microstructures and why trial-and-error methods often remain the industry norm. Indeed, the causes of AGG or CGG could be numerous when considering the applied TM paths and their effect at the microstructure scale. Finally, the concept of the AI-for-AGG proposal will be to move from our simulations' predictive nature to an intuitive understanding of final microstructures characteristics presenting AGG or CGG or even to end up with processing maps exhibiting the windows where the risk of AGG or CGG exists.

This breakthrough objective will be based on our capability to build a massive database concerning available experimental data and numerical predictions of AGG/CGG taken into account all the possible causes and the use of neural network-type algorithms to develop new capabilities on AGG/CGG discrimination and avoidance.

Such a leap in the models will open the door to tune numerically TM routes, build microstructure-targeted processing maps and automatically propose new enhanced homogenized models. AI-for-AGG project brings the cutting-edge and exploding strategies of data science, physically-based models, and machine learning at the service of academic and industrial metallurgy.

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PARTNERS



KEYWORDS

Digital twins - IA - Computational Metallurgy - Grain growth - Deep learning strategy.

CANDIDATE PROFILE AND SKILLS

Degree: MSc or MTech in Applied Mathematics, with excellent academic record. Skills: Numerical Modeling, 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 μ Structure Rheology (MSR) and Computing and Fluids (CFL) research teams under the supervision of Prof. M. Bernacki and Prof. E. Hachem in "Numerical Mathematics, High Performance Computing and Data" doctoral speciality.

[1] M. Bernacki, N. Bozzolo, P. de Micheli, B. Flipon, J. Fausty, L. Maire, and S. Florez, *Recrystallization: Types, Techniques and Applications, ch. Numerical Modeling of Recrystallization in a Level Set Finite Element Framework for Application to Industrial Processes*. Nova Science Publishers, Inc., first edition ed., 2019.

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