M2 Research Internship (6 months)

Assessing the free surface effect in full-field and mean-field numerical simulations of multicrystalline aggregates

Critical mechanical properties of metallic materials are controlled by their **microstructure** and the **relationship between microstructural features and deformation mechanisms** that are activated during service. While high-throughput mechanical testing and material characterization have recently been developed to establish this relationship [1], **numerical simulations** are also a mandatory tool to enable the prediction of mechanical properties. Metallic materials can be very heterogeneous at the micro- and mesoscale (for example in terms of grain sizes, morphologies, crystallographic orientations, etc.) and all these microstructural parameters participate in the local and macroscopic mechanical behaviour of polycrystalline materials.

To predict the overall macroscopic behaviour of the material – which is the main engineering interest, mean-field homogenization methods can be used [2-3]. In these models, the heterogeneity in the microstructure is considered by representing the microstructure as a statistical distribution of microstructural parameters (crystallographic textures, phase morphologies, etc.). The effective behaviour of polycrystals is obtained from the determination of a homogeneous infinite equivalent medium in self-consistent schemes. The main advantage of this method is to offer **reduced computation time and resources** to evaluate the effective response of materials and mean fields within grains (or phases), making it **more applicable in the industry**. However, they lack in correct description of « finite size effects ». Especially, as each grain is considered to be embedded in a homogeneous infinite medium, grains located at or near a free surface (« surface grains ») and bulk grains are not properly distinguished. These free-surface effects can be responsible for a decrease in the mechanical properties of « surface grains », where dislocations can escape through the free-surface due to image forces [4], thus limiting dislocation dynamics and activation of additional slip systems [5].

To take free-**surface effects** into account, full-field numerical simulations can be performed [6]. They are based on an explicit representation of the microstructure (using Representative Volume Elements). They also allow for a **much higher resolution** of microscopic fields (especially the distribution of intragranular stresses and strains) and are **more suitable for the study of complex microstructures** and/or deformation mechanisms. Though, the development of accurate full-field models comes with time- and resource-consuming simulations.

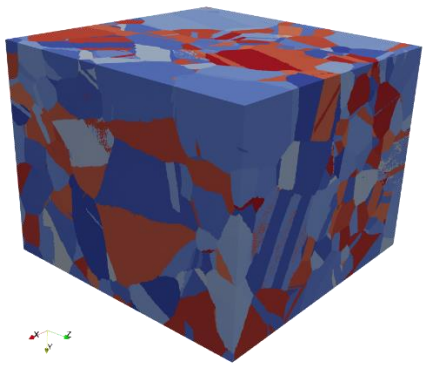

Figure 1: Realistic 3D simulation volume reconstructed from experimental acquisition.

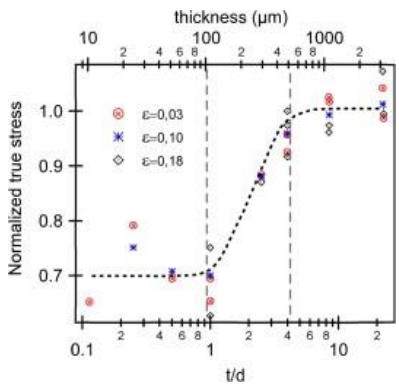

Figure 2: Stress gradient between surface and core grains enhanced with different thickness to grain diameter t/d ratios [5].

In this research project, we aim at studying the free-surface effects through full-field numerical simulations of polycrystalline aggregates at the mesoscopic scale. Also, the main objective is to use these simulations in order to optimize and calibrate new mean-field numerical models at the higher scale specially developed to account for free-surface effects to some extent (e.g. through the computation of three-dimensional Green's functions in half-spaces [7-8]). Full-field numerical simulations will be performed using AMITEX [9], which is a massively parallel solver based on fast Fourier transform for non-linear mechanical simulations on heterogeneous RVE.

The intern will be part of **ERC-Starting Grant HT-S4DefOx** and will interact with different PhD students and postdoctoral fellows involved in this project. Also, the intern will interact with two research teams in two different French laboratories: Institut Clément Ader (CNRS UMR 5312) and LEM3 (UMR CNRS 7239). This internship offer is an interesting opportunity to develop **strong academic and numerical skills** (modelling, micro-mechanics, etc.) to pursue a career in academia or industry.

References:

[1] M. A. Charpagne, J. M. Hestroffer, A. T. Polonsky, M. P. Echlin, D. Texier, V. Valle, J. C. Stinville, Acta Materialia, 2021, 215, 117037.
[2] C. Mareau, S. Berbenni, International Journal of Plasticity, 2015, 64, 134-150 (hal-01513860).
[3] S. Lhadi, S. Berbenni, N. Gey, T. Richeton, L. Germain., International Journal of Plasticity, 2018, 109, 88-107 (hal-02353021).
[4] X. Chen, T. Richeton, C. Motz, S. Berbenni. International Journal of Plasticity, 2021, pp.102967, doi:10.1016/j.ijplas.2021.102967
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[6] M. Sauzay, P. Gilormini, Comptes Rendus de l'Académie des Sciences,-Series IIB-Mechanics-Physics-Astronomy, 2000, 328(2), 117-122.
[7] K.P. Walker, Proceedings of the Royal Society: Math. Phys. Sciences, Vol. 443, No. 1918, 367-389
[8] E. Pan, F.G. Yuan / International Journal of Solids and Structures 37 (2000) 5329±5351
[9] https://amitexfftp.github.io/AMITEX/index.html

Administrative details :

Start : 01/03/2023 for 6 months **Location :** Institut Clément Ader – IMT Mines Albi

- ***Research team and contact information :***

Contacts in hosting lab ICA (Albi, France) :

- **Dr. Julien GENEE** (julien.genee@mines-albi.fr), associate professor, materials science and modeling of material mechanics
- **Dr. Damien TEXIER** (damien.texier@mines-albi.fr), CNRS research scientist, materials science and characterization of high temperature deformation and oxidation

Partners in LEM3 (Metz ; France) :

- **Dr. Stéphane BERBENNI** (stephane.berbenni@univ-lorraine.fr), CNRS research director, expert in continuum modeling of material mechanics
- **Dr. Thiebaud RICHETON** (thiebaud.richeton@univ-lorraine.fr), CNRS research scientist, modeling of material mechanics

- ***Expected skills and interests*** :

Required : good knowledge of materials science (metals), experience with computation languages (Python, Fortran, etc).Please send a detailed CV, an application letter to one the previous contacts.

- ***Application :***

Please send a **detailed CV**, an **application letter**, and **latest grades (L3,M1)** to the emails of the contacts of ICA (Albi, France).