Ph. D. student position open for October 2020

Simulation of plastic strain localization by Discrete Dislocation Dynamics and crystal plasticity

The project 3DiPolyPlast

Understanding the deformation processes leading to the failure of polycrystalline structural materials is one of the key challenges in materials science. Significant progress has been achieved over the past decades, thanks to both cutting-edge experimental characterization techniques and computational methods [1, 2, 3] Still, the localization of plasticity in slip bands and the propagation of plasticity through a polycrystalline aggregate are not fully understood. The investigation of such phenomena is the goal of the ANR project 3DPolyPlast starting in march 2020. The Key objectives of this project are:

1. Pushing the frontier of experimental characterization of bulk plasticity
2. Determining the contribution of slip band/localization in plastic strain of individual grains
3. Identifying mechanisms governing the propagation of plastic strain in the polycrystal
4. Advancing image-based mesoscale modelling of crystal plasticity

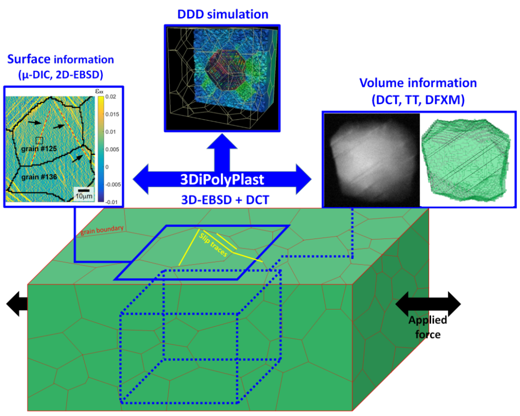

Figure 1: Schematic of the concept of the 3DiPolyPlast project, combining state-of-the-art experimental and simulation techniques into a multi-scale study of the plastic strain localization and propagation in a polycrystalline material.

Ph. D. proposal

Within the 3DiPolyPlast, this open position will particularly focus on objectives 3 and 4. The electron- and synchrotron-based characterizations carried out in the 2 other Ph. D. projects will be compared to the simulation results performed on digital copies ("clones") of the measured 3D grain microstructures. In the proposed multi-scale simulation approach, Discrete Dislocations (DD) simulations will be used in order to better model the individual and collective behaviour of dislocations at the mesoscale. Stress concentration at the origin of strain localization in slip bands is naturally reproduced by DD simulations. Modeling the boundaries in such simulations is non-trivial and will be addressed in the framework of the Discrete-Continuous Model (DCM) which couples crystal plasticity finite element calculations carried out on the full polycrystalline aggregate with DD simulations inside a single grain. This method is based on continuum elasticity theory, which provides the description of the elastic strain field induced by dislocations, their mutual interaction and their interaction with an external stress field [4]. The strong advantage of this method is that stress concentration at the origin of strain localization in slip bands [5] can be accurately simulated by DD calculations.

More specifically, measured 3D grain maps of each sample will be turned into a mesh suitable for DCM and CP-FEM calculations. A classical CP constitutive law will be used in all the grains, but the ones identified experimentally as the grains where first slip bands are recognized. Careful comparison with in situ experiments will be made to validate the fidelity of the DCM simulation and to reproduce the formation of a slip band. In addition, these simulations will provide the mechanical field generated by the slip bands in the vicinity of grain boundaries to analyse the propagation of plasticity from one grain to the next. Repeated simulations with different experimental configurations (grain orientation and boundary conditions for DCM) will be carried out to build a large data set of various micromechanical situations. This work will provide an avenue towards an improved and physically motivated description of crystal plasticity constitutive behaviour for polycrystalline materials.

Informations complémentaires

Timeline 36 months, start October 1st, 2020

Funding ANR Project 3DiPolyPlast

Location Centre des Matériaux, Mines ParisTech – PSL Research University and Laboratoire d'Etude des Microstructures, ONERA Châtillon

Doctoral school ISMME (Ingénierie des Systèmes, Matériaux, Mécanique, Energétique)

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Lien vers l'annonce `https://tinyurl.com/rvftyf8`

Application

Applications are welcomed if your hold a master degree in mechanics of materials or physics. You must show an appetite for large scale simulations of material behaviour and a will to deeply understand the processes behind material deformation. You will be part of a national project regrouping 4 recognized institutes in the field; 3 different PhD student will interact within the project. The Ph. D. candidate is expected to communicate within the project, at relevant conferences and to publish in international journals. Mastering English writing and very good communication skills is mandatory. Please send your application to recrutement_these@mat.mines-paristech.fr

Your application must include: a detailed CV, a covering letter explaining your motivations, all grades obtained during your master degree and the names and contact informations of two person we may contact for recommendation.

References

[1] W. Gerberich et al. Review Article: Case studies in future trends of computational and experimental nanomechanics, *J. Vac. Sci. Technol.* A Vacuum, Surfaces, Film., vol. 35, no. 6, p. 60801, 2017.

[2] L. P. Kubin. Dislocations, mesoscale simulations and plastic flow. In: *Oxford Series On Materials Modelling*, vol. 5, A. P. Sutton and R. E. Rudd, Eds. Oxford University Press, 2013.

[3] U. F. Kocks and H. Mecking. Physics and phenomenology of strain hardening: the FCC case. *Prog. Mater. Sci.*, vol. 48, pp. 171–273, 2003.

[4] B. Devincre and R. Gatti. Physically Justified Models for Crystal Plasticity Developed with Dislocation Dynamics Simulations. *J. AerospaceLab*, vol. 1, pp. 1–7, 2015.

[5] C. Déprés, C. F. Robertson, and M. C. Fivel. Low-strain fatigue in AISI 316L steel surface grains: a three-dimensional discrete dislocation dynamics modelling of the early cycles I. Dislocation microstructures and mechanical behaviour. *Phil. Mag.*, vol. 84, no. 22, pp. 2257–2275, 2004.