PMMH, ESPCI /CNRS – 3 years funded PhD grant

Bridging mesoscopic and molecular scales in crystal plasticity

At Lab. PMMH (www.pmmh.espci.fr), CNRS/ESPCI/Paris 6/Paris 7, Paris, France.

The project aims at building a rigorous connection between the recently proposed mesoscopic tensorial model (MTM) of crystal plasticity [1,2] and the microscale physics of crystal dislocations. The MTM achieves the micro-macro compromise by resolving (in a coarse way) dislocation cores while operating with engineering concepts of stress and strain. It can deal with short-range interactions between dislocations, relies on anisotropic, geometrically nonlinear elasticity, and resolves full crystallographic symmetry, including lattice-invariant shears. It has been shown to deal adequately with the size-dependent response of submicron structural elements and capture the statistical structure of the intermittent acoustic emission generated by plastic flows.

In view of these unique features, MTM is emerging as a major instrument in dealing with plastic response of ultra small systems and with plastic fluctuations. The MTM is based on the fundamental assumption that mesoscale material elements are exposed to an effective tensorial energy landscape that is globally periodic. From the perspective of such Landau-type continuum theory with an infinite number of equivalent energy wells, plastically deformed crystal emerges as a multi-phase mixture of equivalent phases. Despite its unusual for plasticity theory appearance, the model is conceptually very close to the classical continuum plasticity as both theories effectively account for the complexity of energy landscape by introducing low energy valleys describing plastic `mechanisms'.

The main goal of the current project is to quantitatively calibrate the MTM by developing a solid conceptual bridge between atomic and mesoscopic scales. An important step will be the development of rigorous methodological procedure for extracting the mesoscopic parameters from the MD description at atomic scales. Mesoscopic and atomistic simulations will be compared quantitatively for a variety of crystalline materials (FCC, BCC, and HCP lattices) and loading protocols. Several MD potentials corresponding to different crystalline symmetries will be used from the simplest to most realistic ones: Lennard-Jones, EAM, density functional, etc. The calibration of the MTM will also open the way towards systematic comparison with discrete dislocation dynamics (DDD). The goal will be to use the MTM to construct the local rules for DDD which ensure that the latter generates realistic dislocation arrangements even at submicron scale. The ultimate test will be the comparison of the kinetics of microstructure evolution in the two approaches. An important challenge will be to match not only statistics of plastic fluctuations but also to reproduce the shapes of dislocation avalanches.

[1] Landau theory of planar crystal plasticity, R. Baggio, O.U. Salman et al., PRL 123 (20), 205501, 2019
[2] Discontinous yielding of pristine micro-crystals, O.U. Salman et al. Comptes Rendus Physique 22 (S3), 1-48, 2021

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Starting date: October 1st 2023 or later.

Requirements: master degree in nonlinear mechanics, applied mathematics or condensed matter/theoretical physics with interest in general complexity and criticality theory.