Computational Plasticity in crystals and polycrystals

TRACK Number (1000 Computational solid mechanics)

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**Key words:** computational mechanics, multiple scale modelling, plasticity.

ABSTRACT

Material deformation is a core concept in material science and widely applies to all kinds of materials across different length scales, from geo- to nano-, and biologically-inspired materials. Beyond the universal elastic regime, materials deform through lattice defects and local damage at the atomic scale and the formation of dissipative structures, such as grain boundaries and dislocation pileups, ultimately leading to the overall macroscopic plastic deformation at the continuum scale. Plastic deformation poses several challenges to theoretical models and their associated computational methods. By its nonlinear and dissipative nature, it tackles multiple length scales, from the atomistic to the continuum, in systems with different levels of complexity, from single- and poly-crystals to amorphous solids. While for some applications, multiscale approaches are essential to handle microscopic details and macroscopic scales simultaneously, coarse-grained methods are also employed to unveil general features, thus paving the way for focused investigations.

This symposium covers diverse topics on plasticity in single and poly-crystals, and predictability of material deformation in submicron scales where finite-size effects become important. Some of the topics that will be in-focus are dislocation dynamics, size-dependence of fluctuations, predictability of yield stress, grain boundary dynamics, and continuum plasticity models. Particular attention is devoted to different multiscale versus coarse-grained theoretical and computational methods, also involving recent data-based models using machine learning to predict the overall plastic response and yield stress of dislocation networks and microstructures. Analogies among different materials and dedicated applications are also discussed. This symposium gathers experts working on various experimental and theoretical aspects within this field to exchange ideas, outline new challenges, and explore possible collaborations.