Simulation of plastic behavior at different length scales: from the nano- to the macro-scale

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The plastic deformation of metallic materials is a good example of a physical phenomena involving several length scales, from the atomic scale to the macroscale. The origin of plasticity is the collective motion of dislocations causing the slip (and eventually twinning) of the crystallites forming the polycrystalline material. A physically based model of the plastic behavior at any length scale should account for the deformation mechanisms relevant at that length scale. The simulation of that mechanisms involves very different simulation models, from ab-initio or molecular dynamics (MD) for discrete scales to the finite element method for the simulation of macroscopic continuum plasticity. Moreover, the scales are not isolated and the parameters of the models at the relevant length scale could in principle be connected with simulations on a smaller length scale, completing a bottom-up multiscale framework.

In this presentation, a brief overview of the simulation approaches used by the author in the last years to model specific issues of the plastic behavior at different length scales will be presented. It will cover the MD simulation of the void growth process [1] and dislocation movement, the discrete dislocation dynamics simulation of the deformation of a crystal [2,3], the crystal plasticity modeling of crystal indentation [4] and the crystal plasticity finite element simulation of polycrystals [5]. In addition, a multiscale concurrent framework for macroscopic plastic simulations based on polycrystalline mean-field homogenization will be presented [6].

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