Studying Plasticity from the Atomic Scale – Transferring Information between Scales

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Plastic deformation of solids is been traditionally considered on the continuum level, although it has been well known since the pioneering work of Polyani, Taylor and Orowan that microstructural defects on the atomic level is responsible to the macroscopic deformation. However, studying plasticity from the atomic scale is still a great challenge and in order to bridge between gaps in length- and time-scales, multiscale computational approaches are required. In this talk, I will demonstrate sequential multiscale models in which information gained from the atomic scale is being transferred to larger scale simulations. First, I will introduce a dislocation-based constitutive rule for the dynamic strength of metals. The constitutive rule is informed with mobility rules obtained from molecular dynamics (MD) simulations. In addition, thermally-activated dislocation nucleation is implemented in the model. The model is shown to predict accurately the dynamic strength in plate impact experiments at different temperatures. In the second part, I will present an implementation of a cross-slip model in discrete dislocation dynamics (DDD) simulations. Cross-slip is a thermally activated mechanism by which screw dislocations change their glide plane. In particular in face-centered cubic metals, in which dislocations are dissociated, the most common cross-slip mechanism is the Friedel-Escaig (FE), by which dislocations constrict at a point and redissociate in the cross-slip plane. We first constructed a line-tension model, to calculate the free-energy barrier for the cross-slip via the FE mechanism under stress. The cross-slip model was implemented in the DDD code microMegas. We fitted two parameters in the model, the stress-free energy barrier and the attempt rate, to reproduce MD simulations of Cu. We then show that the DDD simulations reproduce the probabilistic behavior of cross-slip in large range of temperature and stresses. An implementation of an atomically-scale cross-slip model allows simulating the microstructure evolution during plastic deformation more accurately.