DISLOCATION DYNAMICS SIMULATIONS AND SCALE TRANSITIONS

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Three lectures will be given in order to highlight the role played by discrete dislocation (DD) simulations in multi-scale modelling of crystal plasticity. DD simulations can indeed fill the gap between atomic simulations (molecular dynamics) and continuum modelling (finite element techniques).

The first lecture will focus on molecular dynamics (MD) simulations dedicated to the study of dislocation behaviour. These simulations are needed to feed DD modelling when elasticity cannot predict some situations. It can be the case for thermally activated mobility of screw dislocations in bcc materials. It is also the case of irradiated materials where dislocations react with Frank loops. Another example concerns dislocation nucleation in confined plasticity like during indentation tests. For all these examples, dislocation reactions can be derived from MD simulations and introduced as local rules in DD codes.

The second lecture will follow the two lectures given by Daniel Weygand who will present the details of DD modelling. We will focus on applications where dislocation dynamics simulations gave concrete results useful for engineering mechanics. Two examples will be presented. The first one deals with fatigue simulations of AISI 316L stainless steel. Simulations performed under various loading and boundary conditions show the crucial role played by cross-slip in the formation of the dislocation microstructure. As the cycling proceeds, slip bands exhibiting well organised dislocation arrangements progressively substitute to dislocation tangles. Calculations of the plastic steps printed on the free surface during the cycling give access to the surface relief which is found to be made of extrusion and intrusion profiles. Analyses of stress and distortion energy concentrations inside the slip bands reveals that a crack would most probably initiate at the surface when multipoles, driven by interfacial dislocations, will reach the surface.
The second example concerns the simulation of nanoindentation tests. This simulation requires coupling DD with FEM in order to enforce the boundary conditions. A nucleation criterion is introduced based on MD simulations. The effect of cross-slip probability on the remaining dislocation microstructure after unloading is analyzed. Indentation size effect, which denotes the decrease of the hardness when the penetration depth in increased, is addressed. Surface relief are analyzed and compared to AFM observations.

The last and third lecture will focus on the transition between DD simulations and continuum mechanics. A set of constitutive equations based on dislocation densities is presented. Each equation is demonstrated from the individual behaviour of dislocation motion in a glide system. Since these equations are based on a physical description of dislocation plasticity, the involved parameters can be identified using DD simulations. The equations are then implanted in ABAQUS in order to perform both explicit and implicit simulations. The continuum model is validated in the case of tensile test of copper single crystals for which the well known three stage curve is reproduced. Finally, FEM simulations of conical indentation are performed in copper crystals of different orientations. Comparisons with experiments give access to the initial dislocation density.