Three dimensional discrete dislocation dynamics modelling: Introduction and Applications

D. Weygand, izbs, Universität Karlsruhe (TH), KIT, Karlsruhe, Germany

The mechanical properties of crystalline materials are determined by the evolution of the dislocation microstructure within the sample. The dislocation motion in small structures is strongly determined by geometrical constraints and often a so called size effect in the flow stress, “smaller is stronger”, is observed. Continuum modelling cannot easily capture size effects, as the characteristic length scale of the dislocation microstructure, e.g. the average spacing between dislocation, and the sample size are too close, and therefore averaging is not allowed. The method of “discrete dislocation dynamics” (DDD) is able to handle this situation, as the motion of the dislocations is explicitly tracked.

The first lecture will give an introduction to the physics of dislocations and their description within linear elasticity theory, needed for the formulation of a discrete dislocation dynamics model. The following points of the model will be detailed:

- geometrical description of dislocation in a DDD model
- basics of dislocation interactions and reactions
- constitutive rules for dislocation motion
- treatment of boundary conditions

The second lecture focuses on applications of discrete dislocation modelling. The stability of specific elementary dislocation interactions will be discussed as well as the interaction of dislocation with obstacle fields both in comparison to MD simulation and to experimental studies. Furthermore the role of dislocation source activation will be discussed, to explain the flow stresses of observed in thin films.

The last series of examples is inspired by numerous studies on the mechanical behaviour of micrometer-sized pillars, produced by FIB (Focused Ion Beam). The DDD method is applied to analyse the size dependency of the measured flow stresses including an analysis of the so-called “strain bursts”, which are a common feature of the stress strain curves. Simulated bending and torsion test are compared to experimental observations and the resulting dislocation microstructure is analysed to explain the observed behaviour.