MM 36: HV Bitzek

Time: Wednesday 14:00–14:30 Location: H16

Invited Talk MM 36.1 Wed 14:00 H16

Atomistic simulations of plastic deformation - insights from a quantitative approach — •Erik Bitzek — Lehrstuhl Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg

Since the first studies on dislocation core structures in the 1960s, atomistic simulations have become an important tool to investigate the mechanical behaviour of materials. Atomistic simulations, for example, allow the direct observation of fundamental dislocation processes like the nucleation of dislocations and their interaction with defects at a length scale where experimental information is difficult to obtain. Besides this kind of *qualitative* studies, atomistic simulations are more and more used in a multiscale modelling framework to provide *quantitative* information on parameters for mesoscopic models like dislocation dynamics simulations. Systematic parameter studies and statistical analysis of atomistic simulations can however provide additional insights, e.g. by revealing correlations between different parameters or by providing a test-bed for (mesoscopic) models.

This talk will provide an overview on parameter studies on dislocations in single crystals, dislocation mediated plasticity in nanocrystals and plastic deformation of metallic glasses by shear transformation zones. The detailed quantitative analyses of the atomistic simulations are compared to current models of nanoscale plasticity.