Atomistic Simulations of Dislocation-Grain Boundary Interactions and Nanocrystal Plasticity

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The mechanical properties of nanocrystalline metals are determined to a large degree by the interaction between dislocations and grain boundaries. The interaction of these lattice defects is governed by processes that take place at the atomic scale. Consequently, atomistic simulations have played a key role in studying the nucleation of dislocations at grain boundaries, as well as their pinning, absorption or transmission through grain boundaries. However, most of the detailed studies on dislocation – grain boundary interactions were performed on quasi-two dimensional set-ups with straight dislocation lines interacting with perfectly planar grain boundaries. Similarly, the deformation of nanocrystalline metals is commonly studied using artificial structures generated by means of the Voronoi tessellation. This procedure creates planar grain boundaries and non-equilibrium triple junction topologies, as well as unrealistic numbers of neighboring grains and distributions of triple line lengths.

Here we present results of controlled studies on dislocation loops interacting with grain boundaries in a bi-crystal using a fully three-dimensional simulation set-up and compare them to the processes taking place during the deformation of various nanocrystalline samples with different degrees of grain boundary curvature as well as different grain boundary network topologies. In addition to the detailed study of dislocation-grain boundary interaction mechanisms, a statistical analysis of the processes contributing to the plastic deformation of the nanocrystalline samples was performed. This analysis provides information on the distribution of critical stresses for dislocation nucleation and dislocation depinning from grain boundaries as well as on the distribution of plastic strain caused by individual slip events. We finally discuss how such an approach can provide valuable parameters for mesoscale models of nanocrystal plasticity like dislocation dynamics simulations or quantized crystal plasticity (QCP).