DIRECT EVALUATION OF DISLOCATION NETWORKS AND DISLOCATION DENSITY TENSORS FROM ATOMISTIC DATA

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Plasticity caused by the nucleation and interaction of dislocations is an important aspect in crystal deformation.
Molecular dynamics simulations offer the possibility to study deformation mechanisms on an atomistic scale without assumptions on strain gradient effects, but require sophisticated analysis routines in order to deal with the large amount of data generated.
A new efficient approach to analyze atomistic data on-the-fly during the simulation is introduced, allowing identification of the dislocation network including their Burgers vectors in high temporal resolution. This data not only provides the evolution of dislocations over time, but enables to quantify dislocation density tensors in three dimensional volume elements with an edge length down to 2 nm. Lattice rotation patterns on an atomic level offer additional information concerning crystal deformation. We have applied these methods in simulations of nanoindentation in single crystal copper and compared the results with experimental data.

The presented approach provides useful insight into deformation mechanisms during plastic deformation and can extract valuable information to bridge simulations on atomic levels and continuum description. Furthermore the methods are easily adaptable to different crystal structures. Besides face centered cubic metals, it has been successfully applied in body centered cubic metals (Fe, W) and multiphase material like austenitic-martensitic shape-memory-alloys.