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FREE ENERGY FUNCTION OF DISLOCATION DENSITIES BY LARGE SCLAE ATOMISTIC SIMULATIONS

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The energy of complex dislocation microstructures is a fundamental property of continuum plasticity on the nanoscale. The question how the energy depends on the characteristic of a dislocation network is still not fully answered, although various - and often contradicting - models have been proposed in the literature.
In this talk, this question is addressed using large scale Molecular Dynamics simulations of nanoindentation, which have been conducted to gain insight into the relationship between dislocation microstructures and the associated free energy from an atomistic level. Several single crystalline samples of aluminum are indented using varying tip radii to study possible size effects. In the largest sample, a 24nm tip is used to indent into a volume of $150^3 nm^3$ that consists of about 2×10^8 atoms. Thus, these atomistic simulations are reaching a size that is comparable to experiments.
Dislocation microstructures are directly identified from the atomistic data, providing the mean to measure both the total and geometrically necessary dislocation densities in the volume and further related them to the energy which is obtained from the simulations as well. Using this approach, an atomistically informed free energy function for dislocation densities is derived from nanomechanical simulations, without the need to account for theoretical or phenomenological arguments commonly used in modeling crystal plasticity.
Furthermore, several size effects are clearly observed in the conducted series of simulations with varying tip radii and sample volumes. Whereas for small indenter tips only plastic deformation by dislocations is observed, twinning and subgrains formation additionally occur in the samples underneath the indenter tips having a radius of 16nm or higher. This mechanism is having a significant influence on the measured geometrically necessary dislocation densities.