

Mechanical models for grain boundaries based on ab-initio results

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The mechanical properties of interfaces determine the strength and deformability of real microstructures. Key quantities like interface energy, work of separation, theoretical shear and tensile strength are important input parameters for mesoscale-simulations of deformation and fracture, and there is a demand for models which can predict the mechanical behavior of interfaces based on these basic properties. Such material parameters can be calculated with high accuracy using ab-initio density functional theory (DFT) methods. Ab-initio calculations also allow a systematic study of the degrees of freedom, such as interface geometry and chemistry. However, this parameter-space is very large and ab-initio calculations are extremely time-consuming. With our studies we are trying to reduce this complexity by looking for correlations between the mechanical properties of grain boundaries and the interface degrees of freedom.

Two applications will be shown in the presentation. The first case describes traction-separation laws for grain boundaries in body centered cubic molybdenum under tensile load. This refractory metal suffers from intrinsic grain boundary brittleness, but experimental studies show that the fracture strength can be greatly enhanced by additions of carbon. Our traction-separation laws take into account the influence of carbon on the interface strength and reproduce the trend which is observed experimentally. In combination with continuum plasticity models, such traction-separation laws can be used in continuum simulations of fracture.

The second example is a potential that describes the coupling of tensile and shear load at different grain boundaries in face-centered cubic aluminum. Similar to the first example, these potentials can be used to derive traction-separation laws for simulation of fracture, this time taking into account different crack propagation modes. On top of that, the characteristic parameters of the potential can be used to evaluate the competition between crack propagation and dislocation nucleation along the grain boundaries. The predictions of our model are verified with molecular dynamics simulations of grain boundary shearing using empirical potentials.