
MM 29: Invited Talk (Hauptvortrag): Janisch

Time: Wednesday 9:30–10:00

Location: H24

Invited Talk

MM 29.1 Wed 9:30 H24

Modelling and understanding the strength of grain boundaries based on ab-initio results — ●REBECCA JANISCH — ICAMS, Ruhr-University Bochum

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. These parameters can be predicted by ab-initio density functional theory calculations with high accuracy. Ab-initio calculations also allow a systematic study of the degrees of freedom, such as interface geometry and chemistry. Unfortunately 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. We are investigating whether there is a relationship between grain boundary energy (or grain boundary work of separation) and the theoretical strength of the interface, and furthermore between the shear strength and the tensile strength of grain boundaries. Unfortunately, according to ab-initio results for different material systems and grain boundary geometries, the answer to the first question is no. However, our results display a unique scaling behavior, which greatly reduces the number of parameters that enter the microstructure-property relationship which we are looking for. Furthermore there seems to be a correlation between tensile and shear strength, which will be discussed against the background of existing grain boundary structure models.