INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Atomistic simulations of fracture in bcc metals: influence of interatomic potential, crack front curvature and grain boundaries on crack-tip plasticity

In this presentation, we address three topics of fundamental importance for understanding the atomic-scale processes leading to crack-tip plasticity in bcc metals: the influences of the used interatomic potential, crack front curvature and grain boundaries.
First, the results of all atomistic simulations depend critically on the model of atomic interaction. We therefore present a systematic study of molecular statics simulations with eight different embedded atom method (EAM) potentials used to simulate mode I fracture in bcc-iron. Comparison of the fracture behavior and critical stress intensity factors to experimental data allows us to rank the potentials according to their capability to realistically model fracture in bcc-iron.
Second, we compare the results for straight crack fronts in two quasi-two-dimensional (2D) set-ups with molecular dynamics simulations of penny-shaped cracks in a three-dimensional (3D) set-up in order to assess the influence of the simulation set-up on crack-tip plasticity. The plastic deformation mechanisms and changes in crack morphology are analyzed in detail and related to the curvature of the crack front and the 3D simulation set-up. The results highlight the importance of 3D models to study crack nuclei and crack-obstacle interactions.
Most materials of technical importance are, however, polycrystals where crack propagation frequently occurs along grain boundaries. For modeling fracture of polycrystalline materials, a detailed understanding of the influence of grain boundary character (misorientation and interface plane) on the fracture behavior is important. We therefore performed atomistic fracture simulations in low-Σ tilt grain boundaries in tungsten and molybdenum bicrystals. In addition to the well-known orientation-depdendent fracture behavior of grain boundaries, our simulations show that the fracture toughness for brittle intergranular fracture (BIF) can also depend on the crack propagation direction and can be significantly larger than the fracture toughness for brittle fracture in single crystals of the corresponding orientation.