MM 25: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and Deformation I

Time: Tuesday 10:15–11:30 Location: BAR 205

Topical Talk MM 25.1 Tue 10:15 BAR 205

Atomistic Studies on the Role of Interface Curvature on Deformation and Failure of Interface-Controlled Materials — •Erik Bitzek — Department of Materials Science and Engineering, FAU Erlangen-Nürnberg

Since processes like crack nucleation and intragranular propagation as well as dislocation nucleation, absorption, transmission or pinning take place at the atomic scale, atomistic simulations have played a key role in studying grain- and interphase boundaries (GBs, IPBs). However, so far most of the studies on the deformation and failure of interface-dominated materials have been performed on simulation setups with planar interfaces.

Here we give an overview on our recent atomistic studies on intergranular fracture and dislocation-interface interactions, with the focus on non-planar boundaries and more realistic GB topologies. Examples include the importance of interface curvature on the misfit dislocation network in realistic microstructures of Ni-base superalloys, studies of slip transmission through curved GBs and the overemphasis or completely suppression of deformation mechanisms in nanocrystalline samples with different degrees of GB curvature.

MM 25.2 Tue 10:45 BAR 205

Machine learning of grain boundaries for property prediction from atomic structure and insights into their atomic building blocks — •Eric Homer[1], Conrad Rosenbrock[2], Gus Hart[2], and Hunter Erickson[1] — [1]Brigham Young University, Department of Mechanical Engineering, Provo, USA — [2]Brigham Young University, Department of Physics and Astronomy, Provo, USA

Big data is a hot topic and is driving innovation in healthcare, logistics, telecommunications, and the automotive industry. It is used in materials science to search for new materials and alloys with unique combinations of properties. We present results of machine learning applied to a large dataset of grain boundaries (GBs) to predict thermodynamic and kinetic properties of materials, including GB energy, temperature-dependent mobility trend, and shear coupling. The machine learning examines the local environment of the atoms and determines similarity metrics, from which it can make predictions. Predictions of GB energy are reasonably accurate, though the accuracy of predictions for the kinetic properties of mobility and shear coupling are lower. Nonetheless, the approach makes reasonable predictions of kinetic properties based solely on the minimum energy structure of GBs. Analysis of the trends in the machine learning data also provide insight into the possible building blocks of GBs, which appear to be a finite set.

MM 25.3 Tue 11:00 BAR 205

Coupling between grain boundary sliding and migration: misorientation dependence — •Askar Sheikh-Ali — Institute of Rheotechnologies LLC, 161-1 Kozhamkulova, 050026, Kazakhstan

Grain boundary sliding behavior has been studied in zinc bicrystals with symmetric tilt boundaries slightly deviated from 123.75°<10-10>Sigma=9 coincidence misorientation. The boundaries span a narrow range of misorientation of 123.6°-131.7°. All investigated boundaries except 131.7°<10-10> boundary demonstrate coupling between grain boundary sliding and migration predicted by DSC-dislocation model. The ratio between boundary sliding and migration is almost the same for all boundaries experiencing coupling between these processes. Sliding along 131.7°<10-10> boundary is not accompanied by regular boundary migration. The transition from coupling to migration free sliding occurred at deviation angle determined by Brandon criterion and was interpreted as a transition from special to general boundaries. Within the accuracy of the experiment, the transition angle remains constant up to the maximum investigated temperature of 400°C (0.97Tm, where Tm is the melting point).

MM 25.4 Tue 11:15 BAR 205

Coupled grain boundary motion driven by elastic anisotropy in FCC Cu — •Christian Brandl — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

Shear-coupled grain boundary motion is one mechanism, where the plastic shear deformation is linked to the microstructure changes by grain growth at low homologous temperatures. The prevailing notion on the driving force on the coupled grain boundary exclusively ascribes a shear stress in the grain boundary as the driving force. Here, we present molecular dynamics simulation to demonstrate coupled grain boundary driving by elastic anisotropy for a general large-angle asymmetry grain boundary in copper. The observed mechanisms is discussed in the framework of general driving forces of interface motion as the reduction of the total free energy grain linked to the defect migration.