MM 53: Interfaces II: Deformation and Motion

Time: Thursday 11:45–12:30 Location: H 0107

MM 53.1 Thu 11:45 H 0107

Atomistic simulation of a severe plastic deformation-induced "high-energy" state of grain boundaries — •Lisa Neier[1], Sergiy Divinski[1], Anantha Padmanabhan[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische-Wilhelms-Universität, 48149 Münster — [2]University of Hyderabad, India

A comparison of microstructures and properties in materials subjected to the later stages of severe plastic deformation (SPD) or steady-state superplastic flow indicates several unexpected similarities especially with respect to the interface response on the deformation, such as grain boundary (GB) sliding events, which lead to a suppression of dislocation activity. Making use of this idea, we propose to describe the experimentally observed "high-energy" (or "non-equilibrium") state of general high-angle GBs in SPD-processed materials in terms of the concept of shear localization in the interfaces. For this purpose, oblate spheroids of a few atomic diameters size have been chosen as the basic units of sliding. By performing atomistic simulations of these special grain boundaries, their response to deformation is analysed. Different properties, as e.g. the coupling of grain boundary motion in normal direction to a shear deformation parallel to the grain boundary or the grain boundary stiffness and the local shear modulus are calculated and compared to those of relaxed high angle grain boundaries.

MM 53.2 Thu 12:00 H 0107

Shearing behaviour of interfaces: linking intrinsic properties with deformation mechanisms — Mansour Kanani, Alexander Hartmaier, and •Rebecca Janisch — ICAMS, Ruhr Universität Bochum, 44780 Bochum

In many interface-dominated nanostructured materials the role of interfaces during deformation is not yet completely clarified. Very fine spacing of interfaces leads to a competition between dislocation controlled and grain boundary sliding based plasticity. To improve our understanding of this competition we have to investigate the atomistic origin of ductility in the interface region. A multi-scale concept is introduced to capture effects of both the electronic and the atomistic level at interfaces in nano-lamellar TiAl alloys. First, we carried out quasi-static calculations of multi-planar generalized stacking fault energy (M-γ) surfaces of the interface plane as well as the adjacent layers. Second, molecular dynamics simulations guided by ab initio γ-surface calculations were carried out for different bicrystal cells under different shear loading conditions. The results show various shear mechanisms such as twin nucleation and migration/absorption, interface partial dislocation nucleation, and rigid grain boundary sliding/migration. The comparison with the M-γ-surfaces allows to create a link between physical properties and deformation mechanisms, and hence between the results of ab-initio calculations and molecular dynamics simulations. Furthermore we discuss the interplay between interface geometry, atomistic structure, and loading conditions, and its impact on the deformability of lamellar microstructures.

MM 53.3 Thu 12:15 H 0107

Molecular dynamics study of the migration kinetics of asymmetric grain boundaries — •Sherri Hadian[1], Blazej Grabowski[1], Christopher Race[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisen Forschung,max planck str 1,Düsseldorf,40237 — [2]The university of Manchester, Manchester, UK

Classical molecular dynamics (MD) simulations are commonly used to explore the migration of grain boundaries. Our previous research on low sigma symmetric boundaries has shown that at conditions of low driving forces as found in actual experimental setups and when going towards system sizes exceeding those commonly employed in MD a novel mechanism becomes operational that is based on mesoscopic island nucleation. [1] In the present study we extend our research towards grain boundaries deviating from the perfect and symmetric arrangement to investigate the kinetics of asymmetric, defective boundaries. Such grain boundaries constitute in fact the majority of experimentally observed moving boundaries. We introduce defects by deviating the boundary plane from a symmetric equilibrium boundary. The results of the simulations show how the fundamental atomistic mechanisms change as the nucleation driven motion shifts towards a step propagating one. [1] - C. P. Race, J. von Pezold, and J. Neugebauer. Phys. Rev. B 89, 214110.