MM 3: Interfaces I: Mechanical properties

Time: Monday 10:15–11:45 Location: H39

MM 3.1 Mon 10:15 H39

Migration mechanisms of grain boundaries deviating from the symmetric tilt orientation — •Sherri Hadian[1], Blazej Grabowski[1], Chris Race[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Dalton Nuclear Institute, University of Manchester, Manchester M13 9PL, United Kingdom

We have studied the migration kinetics and atomistic mechanisms of mixed tilt and twist grain boundaries systematically deviated from the symmetric tilt Σ7 <111> {1 2 3} orientation as they constitute the majority of experimentally observed mobile grain boundaries. Using physically converged simulations and investigating dense motion snapshots in 3D, we find unique characteristic mechanisms in the motion of non-symmetric grain boundaries as compared with the symmetric one. The mixed grain boundaries show nano-faceting, which enables two heterogeneous atomistic migration mechanisms and critically changes the previously reported island nucleation mechanism in the symmetric Σ7 tilt boundary [1]: Depending on the orientation of the nanofacets/steps either a double kink nucleation and propagation or a pure kink flow drives the motion. We show that these atomistic mechanisms are the origin of the observed change from a strongly non-Arrhenius behavior towards a more Arrhenius one and subsequently a change in the asymptotic behavior of the migration barrier at low driving forces as we change the grain boundary from a symmetric tilt to a general mixed one. In the end, connections were made between grain boundary migration processes and those of the surface epitaxial growth.

MM 3.2 Mon 10:30 H39

Shear Modulus of grain boundaries in relaxed and deformation-modified states — •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 properties in materials subjected to severe plastic deformation or steady state superplastic flow shows several similarities especially with respect to the interface response to the deformation, such as grain boundary sliding events. Making use of this idea, we propose to describe the experimentally observed "high-energy" state of general high-angle grain boundaries in severely plastically deformed materials in terms of a concept of shear localization and extra free volume in the interfaces, with oblates spheroids chosen as basic sliding units.

By performing atomistic simulations of these grain boundaries their response to deformation is analysed. With special focus on shear deformation parallel to the grain boundary plane, properties, such as the local shear modulus of these grain boundaries, are calculated and compared to the properties of relaxed high angle grain boundaries.

MM 3.3 Mon 10:45 H39

Atomistic simulations of planar defects in solids: evaluations of present and new methods for computation of strength of grain boundaries — •Petr Šesták[1,2], Petr Řehák[1,2], Miroslav Černý[1,2], Monika Všianská[1,2], Jianying He[3], Jaroslav Pokluda[2], Zhiliang Zhang[3], and Mojmír Šob[1,2,4] — [1]Institute of Physics of Mater., Academy of Sci. of CZ, Brno, CZ — [2]CEITEC, Brno, CZ — [3]Faculty of Engineering Science and Technology, NTNU, Trondheim, NO — [4]Faculty of Science, Masaryk University, Brno, CZ

Planar defects like grain boundaries predetermine mechanical properties of polycrystalline materials and, in particular, their strength. Therefore, a lot of effort has been devoted to study these phenomena not only at macroscopic level but also at nano- and atomistic scales using simulations based on DFT. However, such simulations always omitted the Poisson contraction, which leads to relaxation of transverse stresses. In the present study, we propose and test two models of the tensile tests (including the transverse contraction) on crystals containing planar defects. One model comprises full optimization of the lattice via relaxation of the lateral stress tensor components while the other uses a new, simplified approach. The models are tested and verified for a tensile loading of the Σ5 (210) tilt grain boundary in Ni. The comparison of both methods reveals that the results are almost identical. However, our new model allows us to decrease the computational time significantly. Both models are also compared with former approaches where the Poisson contraction was neglected.

MM 3.4 Mon 11:00 H39

Material transfer and its suppression at Al-TiN and Cu-C interfaces from first principles — •Gregor Feldbauer[1,2,3], Michael Wolloch[2], Pedro 0. Bedolla[3], András Vernes[2,3], Josef Redinger[2], and Peter Mohn[2] — [1]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — [3]AC2T research GmbH, Wiener Neustadt, Austria

Contacts of surfaces at the atomic length scale are of fundamental interest for a better understanding of nanotribological processes, which are crucial in modern applications from nanoindentation or AFM/FFM to nanotechnologies applied in NEMS/MEMS.

A series of density functional theory (DFT) simulations was performed to investigate the approaching, contact and subsequent separation of two atomically flat surfaces consisting of various materials. Here, interfaces between Al and TiN slabs as well as Cu and C (diamond) slabs were chosen as model systems representing the interaction between soft and hard materials. The approaching and separation were simulated by moving one slab in discrete steps and allowing for relaxations after each step. Various configurations of the surfaces were analyzed at the interfaces. Additionally, the effect of oxygen and hydrogen at the Al and C surface, respectively, was investigated. The performed simulations revealed the influences of these aspects on the adhesion, equilibrium distance, charge distribution and material transfer. Particularly, oxygen and hydrogen showed their potential to suppress material transfer at the examined interfaces.

MM 3.5 Mon 11:15 H39

Influence of patterned stress states on Hydrogen loading in Vanadium thin films studied by electrochemical Hydrogenography — •Anshu Tyagi, Florian Döring, Hans-Ulrich Krebs, and Astrid Pundt — Univ. Göttingen, IMP, Friedrich- Hund-Platz 1, 37077 Göttingen, Germany

The mechanical stress state of a metal film sensitively affects the chemical potential of Hydrogen in the metal.[1] The stress state can be changed by the adhesion of the metal film to the substrate.[2] Stress sensitive Vanadium thin films act as model systems in this paper.[3] These films are sputter deposited onto transparent glass substrates. Stress modulation is achieved using patterened Palladium and Polycarbonate layers. The Hydrogen uptake in these films is studied using Hydrogenography which monitors the film transparency and reflectivity.[4] These optical properties depend on the Hydrogen concentration via Lambert-Beer's law. We apply this method using electrochemical loading in a light-microscope. This electrochemical Hydrogenography allows to optically probe for the local Hydrogen concentration. Comparative studies on different adhesion conditions are done by in-situ EMF measurements. This provides the related chemical potentials including information about the phase boundaries. The transmission and reflection spectra are discussed with respect to these data. This research is kindly supported by the DFG via SFB1073 and PU131/9-2. [1] S.Wagner, A. Pundt, APL 92 (2008) 051914. [2] A. Pundt et al. Acta Mater. 52 (2004) 1579. [3] E. T. Gutelmacher et al., J Matter Sci. 45 (2010) 6389. [4] R. Gremaud et al., APL 91 (2007) 231916.

15 min. coffee break