MM 30: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Structure and Deformation II

Time: Tuesday 11:45–13:00 Location: BAR 205

MM 30.1 Tue 11:45 BAR 205

Low angle grain boundaries induced buckling in nanoscale copper films — •Xiaopu Zhang[1], Jian Han[2], David Srolovitz[2], and John Boland[1] — [1]CRANN, Trinity College Dublin, Dublin 2, Ireland — [2]Department of Materials Science and Engineering, University of Pennsylvania, 3231 Walnut St., Philadelphia, PA 19104 USA

Scanning tunneling microscopy is used to study the grain boundaries that emerge at the surface of nearly coplanar copper nanocrystalline films with (111) surface orientations. At symmetric low angle grain boundaries the film is found to buckle so as to form valleys comprised of dissociated edge dislocations and ridges where dislocations have recombined. Geometry analysis shows that buckling is induced by the out-of-plane grain rotation driven by the favorable energy of dislocation-dissociation, and confirmed by simulations. Due to the symmetry of the FCC slab, both the type of emergent grain boundaries (dissociated or recombined) and the film buckling sense are forced to toggle whenever grain boundaries shift direction by 60o, producing a novel buckling pattern. These results indicate that it is impossible to form perfectly flat two dimensional nanoscale films of copper and indeed other metals that exhibit low dislocation-dissociation energies.

MM 30.2 Tue 12:00 BAR 205

Tensorial elastic properties and stability of interface states associated with Σ5(210) grain boundaries in Ni_3(Al,Si) — •Martin Friák[1,2], Monika Všianká[2,1], David Holec[3], and Mojmír Šob[2,1,4] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Grain boundaries (GBs) represent one of the most important types of defects in solids. They are challenging for theoretical studies because of their distorted atomic structure. We use *ab initio* methods to assess tensorial elastic properties of interface states associated with GBs. Focusing on the Σ5(210) GBs in Ni_3Al intermetallics as a case study, we evaluate the mechanical stability of the interface states by checking Born-Huang's stability criteria. The elastic constant C_{55} is found three-/five-fold lower than in the bulk and, as a result, the mechanical stability of interface states is reduced. The tensorial elasto-chemical complexity of the interface states is demonstrated by a high sensitivity of elastic constants to the GB composition. In particular, we study elasticity changes induced by Si atoms segregating into the atomic layers close to the GBs and substituting Al atoms. If wisely exploited, our study paves the way towards solute-controlled design of GB-related interface states with tailored stability and/or tensorial properties.

MM 30.3 Tue 12:15 BAR 205

Grain boundary strain accommodation mechanisms in ultrafine-grained Pd — •Yulia Ivanisenko[1], Nariman A. Enikeev[2], and Kejing Yang[3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, 450000 Ufa, Russia — [3]Robert Bosch GmbH, AE/EAI2, D71701 Schwieberdingen, Germany

The role of non-crystallographic deformation modes such as grain boundary sliding and rotation in plasticity of ultrafine-grained materials (UFG) is still a matter of discussion. In general, it is assumed that such strain accommodation is considerable at grain sizes in the range of a few tens of nanometers while for the larger grains dislocation-based mechanisms operate. In situ SEM compression test was performed on UFG Pd sample with a mean grain size of 135 nm and orientations of statistically sound sampling of grains were monitored. In order to separate the effects related with dislocation slip, the modeling of the evolution of grain orientations under compression using the methods of crystal plasticity simulation were performed. The analysis of the results shows that grain boundary sliding and non-crystallographic grain rotations contribute considerably to the plasticity of UFG materials. The grains tend to slide and to rotate in a group mode, which testifies to collective character of grain boundary deformation mechanisms in UFG Pd. It was proposed that such grain rotations provide a mechanism for the accommodation of the strain incompatibility between neighboring grains arising during straining.

MM 30.4 Tue 12:30 BAR 205

Energetics of deformed As, Sb and Bi and local deformation of overlayers at interfaces with various substrates — Martin Zouhar[1] and •Mojmir Sob[1,2,3] — [1]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [3]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We present a comprehensive density-functional theory study of total energy and structural properties of As, Sb and Bi in their A7 ground-state structure and in the bcc, fcc and simple cubic (sc) modifications. We also investigate continuous structural transitions between these structures. The total energies of deformed structures are displayed in contour plots as functions of selected structural parameters and/or atomic volume; these plots are then used for understanding and interpreting structural parameters of As, Sb and Bi overlayers on various substrates. Our calculated values of lattice parameters for (0001) thin films of Bi on Si(111) and Ge(111) substrates agree very well with available experimental data. In analogy with that, we suggest to investigate (0001) overlayers of As on Ti(0001), Co(0001), Zn(0001) and Rh(111) substrates, of Sb on C(0001), Zn(0001), Al(111), Ag(111) and Au(111) substrates and of Bi on Co(0001), Al(111), Rh(111), Ba(111) and Pb(111) substrates. For these cases, we also predict the lattice parameters of the films. A large part of our results are theoretical predictions which may motivate experimentalists for a deeper study of these systems.

MM 30.5 Tue 12:45 BAR 205

Deformation behavior in multilayered thin films with different interface structures under sliding contact — •Ankush Kashiwar[1], Zhao-Ping Luo[2], Ruth Schwaiger[1,3], and Christian Kübel[1,3] — [1]Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Shenyang National Laboratory for Materials Science, Shenyang 110016, China — [3]Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

The presented study aims at investigating the deformation structure under sliding contact in multilayered systems with different interface structures. Cyclic sliding experiments were performed on sputtered nanocrystalline metallic multilayers with semi-coherent (Au/Cu) and incoherent (Cu/Cr) interfaces. The deformed microstructure was investigated using automated crystal orientation mapping (ACOM) in a transmission electron microscope. It is revealed that Au/Cu multilayers with a high density of twins deform by de-twinning and grain growth with a simultaneous vortex-like co-deformation and mechanical intermixing between Au and Cu layers. In case of Cu/Cr multilayers, a significant grain growth is observed in all the Cu layers and the grain size increases with the increasing number of loading cycles, whereas there is no noticeable change in the grain sizes in the Cr layers. Unlike Au/Cu multilayers, the phase maps show sharp boundaries between Cu and Cr layers, indicating no intermixing between the layers.