MM 39: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Grain Boundaries and Nanoporous Materials

Time: Wednesday 15:15–16:45 Location: H 0107

MM 39.1 Wed 15:15 H 0107

Observation of dislocation interactions with an asymmetric grain boundary in Cu by high frame-rate in-situ TEM — •Nicolas J Peter[1], Vasfi B Özdöl[2], Colin Ophus[2], Chrsitian H Liebscher[1], Christoph Kirchlechner[1], Andrew Minor[2], and Gerhard Dehm[1] — [1]Max-Planck Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]National Center for Electron Microscopy, Berkeley, USA

In-situ TEM nanomechanical testing enables direct visualization of plasticity mechanisms for deformation experiments at small scales. For instance, dislocation source operation and dislocation-dislocation interactions were studied in single crystalline materials to resolve the mechanisms controlling size scaling effects. However, far less studies are focused on unraveling dislocation interactions with interfaces, although understanding these plasticity mechanisms is important for structural materials. In the present study the atomic grain boundary structure of an artificially grown bicrystal was characterized by high-resolution STEM. Nano pillars containing the boundary and from adjacent grains were FIB-machined and tested in-situ inside a TEM equipped with a direct electron detector at a framerate of 400 fps. Fully and partially annealed samples were tested to investigate and reduce the impact of FIB damage that strongly affects the initial dislocation densities. Stable dislocation loop emission and dislocation glide were found to be main plasticity features in the single crystal references. Dislocation absorption, emission and pinning at the grain boundary were observed in the bicrystals and will be discussed in the talk.

MM 39.2 Wed 15:30 H 0107

Grain Boundary Effects in a High Entropy Alloys: Insights from Atomistic Computer Simulations — •Daniel Utt, Alexander Stukowski, and Karsten Albe — FB Materialwissenschaft FG Materialmodellierung, Technische Universität Darmstadt, Deutschland

High entropy alloys (HEAs) contain principle elements in concentrations between 5 and 35 at.%. Here we investigate the equimolar model alloy CuNiCoFe using atomistic simulations. We employs the embedded atom method potential by Zhou et al. (PRB **69**, 2004), which has been used for HEA simulations before, but was not characterized further. We systematically determine thermodynamic properties of all binary subsystems, with a focus on mixing enthalpies of random solid solutions, and confirm its validity. [Koch et al. (JAP **122**, 2017)]. We investigate the grain boundary (GB) segregation behavior in bicrystalline $Cu_x(NiCoFe)_{1-x}$ samples using a hybrid Monte Carlo / Molecular Dynamics algorithm. We discover significant Cu segregation at these GBs and show that the McLean model is not capable of describing GB segregation in this psudobinary system. Opposite to that, we find, that there is no segregation to planar defects like stacking and twinning faults. Further, we investigate nanocrystalline samples and discover that the HEA is much more resilient against thermal and stress-driven grain growth than elemental elemental nanocrystalline Cu or Ni. Comparing the grain growth and yield strength of a Cu segregated and truly random nanocrystalline CuNiCoFe HEA sample shows no significant influence of the Cu enrichment.

MM 39.3 Wed 15:45 H 0107

Tensorial elastic properties and thermodynamic stability of Σ5(210) grain-boundary interface states in Ni_3Al — •Martin Friák[1,2], Monika Všianská[1,3,4], David Holec[5], and Mojmír Šob[3,1,4] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [5]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, Leoben, Austria

Grain boundaries (GBs) are among the most important defects in solids and their properties are crucial for many materials properties including their (in)stability. We calculate and analyze (tensorial) anisotropic elastic properties of interface states associated with GBs in Ni_3Al. Selecting the Σ5(210) GBs as a case study, we address the mechanical stability of the GB interface states by checking elasticity-based Born stability criteria. One of critically important elastic constants, C_{55}, is found three times lower than in the bulk. Having the complete elastic tensor of Σ5(210) GB states we combine a Green's-function based homogenization techniques and an approximative approach to the Debye model to compare thermodynamic properties of a perfect Ni_3Al bulk and the Σ5(210) GB states. A significant reduction of the melting temperature is predicted (see IOP Conf. Series: Mat. Sci. Eng. 219 (2017) 012019 doi:10.1088/1757-899X/219/1/012019).

MM 39.4 Wed 16:00 H 0107

Mechanical properties of nanoporous gold - impact of solid fraction — •Birthe Zandersons[1], Lukas Lührs[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]InstitInstitute of Materials Physics and Technology, Hamburg University of Technologyute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Nanoporous gold (NPG) is an attractive model system for studies of small scale mechanical behavior. Its centimeter-sized open porous bodies are structured by a monolithic network of struts or "ligaments". The ligament size can be tuned in the range of a few to several hundred nanometer. In the last years several studies find the mechanical behavior of NPG reproducible and highly consistent, except that the results fall in groups of substantially different strength. A widespread theory connects these differences to the variation of solid fraction due to different preparation. Here, we present a systematic investigation of the influence of preparation for the mechanical properties of NPG, using the most common preparation methods. Precursor alloys Au_xAg_{100-x} with $x = 20, 25, 30, 35$ are dealloyed electrochemically in 1 M $HClO_4$ and with free corrosion in concentrated HNO_3. Using continous loading and load/ unload compression tests we investigate the stress-strain behaviour, Young's modulus and Poisson's ratio and confirm substential differences depending on the initial alloy composition.

MM 39.5 Wed 16:15 H 0107

Effect of Polypyrrole Coating on the Elasticity of Nanoporous Gold — •Jie Li[1], Nadiia Mameka[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Dealloying-derived millimeter-size nanoporous gold (np-Au), consisting of interconnected single nanoligaments network with large surface area, exhibits a switchable elastic modulus when its surface is electrically polarized in aqueous electrolyte [1]. Here, we decorate the surface of np-Au by a conductive polymer polypyrrole (PPy) that is also known to exhibit tunable Young's modulus upon charging in electrolytes [2]. While keeping the original porous structure, we have achieved a uniform PPy coating of various thicknesses in bulk np-Au by electropolymerization. The np-Au/PPy composites are then infiltrated by an aqueous electrolyte and subjected to potential variation in dynamic mechanical analyzer (DMA). The in situ DMA experiments reveal that the stiffness variation reaches the same magnitude as in the oxidation/reduction regime on pure gold without polymer coating. The material softens upon negative charging. We discuss possible mechanisms for the stiffness variation. [1] Mameka et al , Acta Mater. 76 (2014) 272. [2] Shoa et al, Synthetic Mater. 160 (2010) 1280.

MM 39.6 Wed 16:30 H 0107

Self-assembled monolayers of alkanethiols strengthen nanoporous metal — •Nadiia Mameka[1], Hartmut Gliemann[2], Jörg Weissmüller[1,3], and Christof Wöll[2] — [1]Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [3]Hamburg University of Technology, Hamburg, Germany

As one of the consequences of the large specific surface area of nanoporous metals, their mechanical behavior is sensitive to the surface chemistry. Studies on nanoporous gold (NPG) modified by a molecular monolayer of OH^- ions exemplify this, finding two-fold increase of

strength [1] and 8% increase of stiffness [2].

Here, we employ self-assembled monolayers (SAMs) of alkanethiols to modify NPG surface. Alkanethiol molecules, consisting of a sulfur headgroup that strongly interact with a metal substrate, a hydrocarbon chain and end-group, are known to spontaneously self-organize into well-ordered, dense two-dimensional molecular films. Alkanethiols with various chain lengths and terminal groups were used to prepare SAMs on bulk NPG and compression tests were performed on the SAM-modified and non-modified macroscopic samples. Our experiments reveal the substantial strengthening of the material due to the thiol adsorption that can reach up to 40%. This talk will discuss possible strengthening mechanisms mediated by the metal-sulfur interaction.

[1] Jin, Weissmüller, Science, 332 (2011) 1179. [2] Mameka et al, Acta Materialia, 76 (2014) 272.