MM 8: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Segregation and Embrittlement II

Time: Monday 11:45–13:15 Location: BAR 205

MM 8.1 Mon 11:45 BAR 205

Atomistic study of Hydrogen embrittlement of grain boundaries in Nickel — •Ali Tehranchi and William A. Curtin — Laboratory for Multiscale Mechanics Modeling, EPFL, CH-1015 Lausanne, Switzerland

The Hydrogen ingress into a metal is a persistent source of embrittlement. Fracture surfaces are often intergranular, suggesting favorable cleave crack growth along grain boundaries (GBs) as one driver for embrittlement. Here, atomistic simulations are used to investigate the effects of segregated hydrogen on the behavior of cracks along various symmetric tilt grain boundaries in fcc Nickel. The results of the simulations are compared with the theoretical predictions of Rice and Griffith theories. Both simulations and theoretical calculations showed that the presence of segregated hydrogen atoms cannot transform the ductile behavior of an intrinsically ductile crack to brittle behavior. For the intrinsically brittle cracks, hydrogen atoms decrease the critical cleavage load. Thus cleavage-like failure observed in the experiments are presumably caused by mechanisms involving H diffusion or dynamic crack growth.

MM 8.2 Mon 12:00 BAR 205

Defect generation in Palladium by Hydrogen loaded Niobium layers — •Vladimir Burlaka, Vladimir Roddatis, Marian Bongers, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Germany

In this paper, we use layers with high hydrogen affinity to influence the defect structure of an overlaying catalytic layer. It will be shown that pre-existing defects can be healed out by a low-pressure hydrogen treatment and, opposite, additional defects can be generated by a higher pressure treatment. In our study Pd/Nb/Al2O3 double layers are studied during hydrogen gas exposure at room temperature by using Scanning Tunneling Microscopy (STM), X-ray diffraction (XRD) and environmental transmission electron microscopy (ETEM). [1] STM results show hydrogen-induced topography changes at the Pd/Nb interface. The XRD measurements demonstrate that the topography changes in the Nb-H film result in microstructural changes in the overlaying Pd layer. ETEM measurements on cross-cut lamellas show that the modification of the Pd top-layer occurs due to the precipitation and growth of the hydride phase within the Nb underlying film: generation of new defects and interface roughening are observed. We conclude that these changes in the Pd layer can be varied by changing the Nb-film thickness. [2]

Financial support by the DFG via PU131/9 and PU131/12 and the beamtime provided by DESY and ESRF are acknowledged. [1] V.Burlaka, S.Wagner, M.Hamm, A.Pundt, Nano Letters 16 (2016) 6207. [2] V.Burlaka, V.Roddatis, M.Bongers, A.Pundt, submitted.

MM 8.3 Mon 12:15 BAR 205

Confined topological impurity segregation at faceted Si grain boundaries — •Christian Liebscher[1], Andreas Stoffers[1], Oana Cojocaru-Mirédin[2], Baptiste Gault[1], Christina Scheu[1], Gerhard Dehm[1], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]RWTH Aachen, Institute of Physics (IA), 52056 Aachen, Germany

Coincident site lattice (CSL) boundaries and trace impurities of Carbon (C) and Iron (Fe) are degrading the electrical performance of multicrystalline Silicon (mc-Si) by promoting charge carrier recombination. Our study provides unprecedented insights into the connection of the faceted nature of grain boundaries in mc-Si and confined impurity segregation. The direct correlation of atomic resolution aberration-corrected scanning transmission electron microscopy (STEM) and 3D atom probe tomography (APT), obtained by probing exactly the same specimen position in both instruments establishes segregation of Carbon (C) and Iron (Fe+N) to linear junctions of merging grain boundary facets. Both, the segregation patterns of C and (Fe+N), as observed by APT, form linear segregation tubes that decorate facet junctions of a $\Sigma3$ grain boundary with a facet length between 2 and 10 nm. By observing the atomic structure of a $\Sigma9$ grain boundary with a facet length of 10 to 50 nm on an APT needle by STEM followed by subsequent 3D chemical analysis directly verifies the confined impurity segregation that is driven by the grain boundary topology.

MM 8.4 Mon 12:30 BAR 205

stInvestigations on Grain boundary Segregation in Nanocryalline Materials with Atom Probe Tomography — •Rüya Duran and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

Nanomaterials are not just opening new opportunities for improvement of materials, but also challenges in characterizing and understanding the changed atomic structures and the chemical and physical behavior within the material. Grain boundaries have the major influence on the properties. An important property is the segregation at these defects. The grain boundary interacts with solute atoms which change their chemical composition and change the boundary and so, the material properties. In this work, the temperature and concentration dependence of grain boundary segregation in Cu/Ni thin films is investigated. For the analysis the Atom Probe Tomography (APT) is used. With the APT a very high spatial resolution in all three dimensions is achieved which makes the analysis of such a fine defect more precise. Since the APT allows chemical analysis in single atom sensitivity, segregation to grain boundaries can be easily identified. With the knowledge of the chemical composition, concentration profiles can be formed from which the widths and also the amplitudes of the segregation zones can be determined. With a new evaluation method the data will be extracted by using a model function for the defect which is fitted to the point data to increase the spatial resolution and to avoid artefacts.

MM 8.5 Mon 12:45 BAR 205

Macroscopic and microscopic investigation of Sulphur - induced embrittlement in Copper — •Thorsten Meiners, Zirong Peng, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Sulphur (S) is a common impurity element, which has a very low solubility in copper alloys (Cu) and is attributed to cause grain boundary (GB) embrittlement by segregating to the boundaries. In our study, macro-tensile tests at room temperature (RT), 200 °C and 400 °C are applied to investigate embrittlement of polycrystalline Cu alloys containing 14, 27 and 7900 ppm of S, named alloy 1, 2 and 3 here. Alloy 1 shows a reduction in ductility of 18% from RT to 400 °C. Compared to that, alloy 2 shows a reduction in ductility of 29% at RT and 70% at 400 °C and alloy 3 58% at RT and 67% at 400 °C. The grain size was determined to about 2 mm using electron backscatter diffraction. Alloy 1 is free of precipitates and high resolution transmission electron microscopy (TEM) and atom probe tomography reveal no segregation of S to random GBs. In alloy 2, small precipitates on the order of 50nm can be established at the GBs and within the grains with scanning electron microscopy. Alloy 3 shows a dendritic structure where large low chalcocite Cu2S precipitates (several micro meters) are located at the dendrites and small precipitates (about 50 nm) are located in interdendritic regions. For the alloys 2 and 3 high-resolution TEM does also not confirm segregation of S to the random GBs and the embrittlement of the alloys is mainly related to the presence of precipitates.

MM 8.6 Mon 13:00 BAR 205

Silver segregation induced nanofaceting of an asymmetric tilt grain boundary in copper — •Nicolas J. Peter, Christian H. Liebscher, Raheleh Hadian, Blazej Grabowski, Christoph Kirchlechner, and Gerhard Dehm — Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Grain boundary faceting is a thermally activated process. It can be suppressed on experimental time scales depending on temperature and driving force. We show here that chemistry can be used to intentionally trigger faceting.

The present study investigates the segregation of Ag to an asymmetric tilt boundary in Cu. Aberration-corrected high-resolution scanning transmission electron microscopy reveals that annealing the Ag coated bicrystal at 800°C for 120 h results in the formation of nanometer-sized, regularly spaced, symmetric Sigma 5 (210) segments within the overall asymmetric boundary. We confirm that reference samples without Ag, annealed under the same conditions, show no thermally activated faceting, even down to the atomic level.

Our observations oppose an anticipated trend to form coarse facets or change the overall boundary plane orientation to lower energy Sigma 5 (210) or (310) planes. Atomistic simulations on specifically chosen reference boundaries support the experimental observations and reveal the atomistic mechanisms of the chemically induced nanofaceting.

Migration paths and atomic column occupancies are extracted over time to allow for a first quantification approach of such a system, thereby showing the stability of the induced Ag containing nanofacets.