MM 18: Interfaces

Time: Tuesday 14:15–15:30 Location: H45

MM 18.1 Tue 14:15 H45

Influence of Ta and Zr segregation on the atomic structure of [111] tilt grain boundaries in Copper — •Thorsten Meiners, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Recently, nanocrystalline Copper (Cu) has been investigated intensively, because of its excellent properties such as high strength and hardness. However, at elevated temperatures rapid grain growth causes a destabilization of the microstructure. Therefore, alloying Cu with immiscible elements such as Zr and Ta has shown to greatly stabilize the microstructure induced by strong grain boundary (GB) segregation and precipitation. In our study we investigate the atomic structure of these GB segregation and precipitation phenomena at [111] tilt GBs in Cu by aberration-corrected (scanning) transmission electron microscopy in order to identify the atomistic mechanisms of the microstructure stabilization. We found spherical Ta_{x}O nano particles at the GBs, which locally distort the GB plane and can thus lead to Zener pinning. Zr is found to form a kind of glass-phase, which is inhomogenously distributed at the GBs. Especially GB steps are strongly decorated with nanometer sized Zr-rich inclusions. In addition we observe Zr-induced structural transitions compared to clean GBs, indicating that these local chemical states alter the GB properties.

MM 18.2 Tue 14:30 H45

Partitioning of segregating impurities during grain boundary decohesion — Xiang Huang[1,2], Alexander Hartmaier[1], and •Rebecca Janisch[1] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]Department of Chemistry, Technical University Munich, Germany

The embrittling effect of hydrogen atoms at grain boundaries is widely studied by means of density functional theory calculations. A first indicator on the effect of H on the interface cohesion is the change in the work of separation due to the impurity. The work of separation is simply the difference between the energy of the two free surfaces after a brittle cleavage of the interface, and the grain boundary energy. However, in the case of a grain boundary with segregated impurities and/or alloying atoms, several possibilities exist of how to distribute the segregants on the two surfaces. In this work we demonstrate the striking effect of different partition patterns and additional surface diffusion on the final effect of C and H atoms on the cohesive behavior of a bcc Fe $\Sigma3(112)[110]$ symmetrical grain boundary. The change in the work of separation is further analyzed by decomposition into chemical and mechanical contribution according to the thermodynamic theory of Rice and Wang.

MM 18.3 Tue 14:45 H45

Amorphous interlayers in semiconductor metallization — •Dennis König, Efi Hadjixenophontos, Guido Schmitz, and Kevin Treder — Institute of Materials Sience, Chair of Material Physics, University of Stuttgart, Heisenbergstraße 3, 70569, Germany

Deposition of thin metallic films on monocrystalline silicon substrates has been extensively used in the past. An amorphous interlayer of few nm, between the silicon and the metallic coating is reported in such systems. During this work detailed investigation on this interlayer is done. Different parameters are studied such as: The cleaning time of the substrates, the power during deposition and the metallic element (Al, Au and Ag) in contact with the substrate. Samples are prepared by Ion beam sputtering with controlled thicknesses and are characterized by HRTEM after FIB cross sections. Further elemental analysis is done by EDX during microscopy. A clear dependency of the thickness of interlayer is observed on the cleaning time and power during deposition. Attempts to identify the composition of the amorphous interlayer are performed by Atom Probe Tomography.

MM 18.4 Tue 15:00 H45

A quantum-mechanical study of connections between tensorial elastic properties and chemical bonds in $\Sigma5(210)$ grain boundaries in Ni_3Si compound — •Martin Friák[1], Martin Zelený[2,3], Monika Všianská[4,1,5], David Holec[6], and Mojmír Šob[5,1,4] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Institute of Materials Science and Engineering, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Faculty of Mathematics and Physics, Charles University in Prague, Prague, Czech Republic — [4]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [6]Department of Materials Science, Montanuniversität Leoben, Leoben, Austria

Using *ab initio* methods we calculate and analyze (tensorial) anisotropic elastic properties of interface states associated with $\Sigma5(210)$ grain boundaries (GBs) in cubic $L1_2$-structure Ni_3Si. In particular, we show that GB variant containing both Ni and Si atoms at the interface is unstable with respect to a shear deformation (one of the elastic constants, C_{55}, is negative). Our elastic-constant analysis allowed us to identify a shear-deformation mode reducing the energy and eventually to obtain mechanically stable ground-state. We further discuss an atomistic origin of this instability in terms of the crystal orbital Hamilton population (COHP) and phonon dispersion calculations. For details see Friák *et al.* Materials 11 (2018) 2263.

MM 18.5 Tue 15:15 H45

Size independent description of the strain effects on the segregation of carbon and hydrogen in iron — •Abril Azócar Guzmán, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-Universität, Bochum, Germany

Structural materials such as steels are frequently processed under stress and strain conditions; in such systems, C and H have been shown to strongly affect the mechanical properties of Fe. Therefore, it is of interest to understand the coupling between segregation phenomena and mechanical response. In this work, we study the cohesion behaviour of a $\Sigma5(310)[001]$ symmetrical tilt grain boundary (STGB) in body centred cubic (bcc) Fe with C as an interstitial alloying element and H as an impurity. Using first-principles calculations, the solution and segregation energies are obtained for varying mechanical load and GB coverage of the segregating atoms, either for fixed concentration or fixed chemical potential. Thus, the maximum concentration of C and H is calculated. We discuss that the concept of strain, or displacement, in *ab initio* tensile tests that include structural relaxations is ill-defined due to the release of elastic energy, which causes the calculated total energies to depend on the system size. The proposed procedure is to obtain the solution energies as a function of the stress instead of the displacement (or strain), assuming that the stress distributes equally among crystallographic planes in the supercell.