MM 3: Topical Session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Segregation and Embrittlement I

Time: Monday 10:15–11:30 Location: BAR 205

Topical Talk MM 3.1 Mon 10:15 BAR 205

Tensile strength in ab initio simulations: stability of models with planar defects — •Petr Šesták[1,2], Miroslav Černý[1,2], Monika Všianská[1,2], and Mojmír Šob[1,2,3] — [1]Institute of Physics of Mater., Academy of Sci. of CZ, Brno, CZ — [2]Central European Institute of Technology, Brno, CZ — [3]Faculty of Science, Masaryk University, Brno, CZ

Ab initio simulations represent an efficient way how to study material properties in those cases where experimental methods are too expensive or impossible to use. However, periodic boundary conditions employed in such simulations impose severe limitations to the size of the simulation cell that can contain just a few hundred atoms at the most. Correct design of appropriate computational cells and simulation models is then a crucial issue in applications of ab initio approaches in simulations of defects.

Here we provide a critical comparison of several models often used for determination of the tensile strength of crystalline systems with planar defects (such as the Σ3 (111), Σ5 (210), Σ5 (310) and Σ11 (311) grain boundaries in fcc nickel) and interfaces in selected composites. Special attention is paid to differences in predictions of individual models and to their sensitivity to the size of the simulation cell (i.e. to different density of defects).

MM 3.2 Mon 10:45 BAR 205

Engineering the chemistry of grain boundaries in Mo-Hf alloys — •Daniel Scheiber[1], Katharina Leitner[2], Reinhard Pippan[3], Peter Puschnig[4], and Lorenz Romaner[1] — [1]Materials Center Leoben, Austria — [2]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Austria — [3]University of Graz, Institute of Physics, Austria — [4]Erich Schmid Institut of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Molybdenum alloys are known for their outstanding material properties like low thermal expansion coefficients and high strength at elevated temperatures. However, many Mo alloys are prone to brittle intergranular fracture at room temperature, which is attributed to low grain boundary (GB) cohesion. GB engineering searches for ways to counteract the low GB cohesion, e.g. by alloying with elements that segregate to the GB and enhance GB cohesion. In this study, Mo samples with different Hf contents are investigated, which exhibit a change from intergranular fracture to transgranular fracture with increasing Hf content. To reveal the underlying effects of this change in fracture mode, different experimental and theoretical methods are applied. A detailed atom probe tomography (APT) study shows the change in GB chemistry for the alloys and clarifies that not Hf, but rather segregated B and C atoms lead to the increase in GB cohesion. Subsequent ab-initio simulations of a GB observed in APT allows for comparison of the GB chemistry with experiment. With the agreement at hand, the simulations explain the change in GB chemistry and provide recommendations for Mo alloys with reduced intergranular fracture.

MM 3.3 Mon 11:00 BAR 205

Influence of hydrogen on grain boundary cohesion in nickel — •Matous Mrovec[1,2], Davide Di Stefano[2], Benedikt Ziebarth[2], and Christian Elsässer[2] — [1]ICAMS, Ruhr-Univerität Bochum — [2]Fraunhofer IWM, Freiburg

The presence of hydrogen in metals often leads to marked lowering of their ductility, fracture strength and fracture toughness - a phenomenon commonly known as hydrogen embrittlement (HE). One of possible HE mechanisms is related to segregation of hydrogen at grain boundaries (GBs) that weakens the GB strength and results in easier intergranular decohesion. It has been observed that the susceptibility to hydrogen-induced intergranular embrittlement varies for different microstructures and hydrogen concentrations. However, quantitative knowledge of key quantities such as hydrogen binding energies at various GBs or critical hydrogen concentrations for fracture is still limited.

In this theoretical study, we explore the interaction of H with several grain boundaries in Ni at the atomic scale using first principles calculations based on density functional theory (DFT). We calculate H diffusion barriers and segregation energies in the vicinity of the GBs and relate these quantities to the geometrical characteristics of structural units composing the GBs. In addition, we also investigate the influence of H concentration on the cohesive behavior of the investigated GBs and compare the theoretical predictions with existing experimental results.

MM 3.4 Mon 11:15 BAR 205

Effects of alloying elements on H embrittlement of C segregated grain boundaries in bcc Fe — •Aparna P. A. Subramanyam, Abril Azocar Guzman, Xiang Huang, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr University-Bochum, Bochum, Germany

The cohesion of grain boundaries (GBs) is dependent on their chemical composition and structure and greatly influences the mechanical properties of the material. It is well known that H prefers segregating to the GBs (and other defects). H enhanced decohesion is one important mechanism of H embrittlement. Therefore it is necessary to understand the effects of alloying additions on the segregation behaviour of H and on the embrittling mechanism.

The embrittling effects of H in the presence of alloying elements Mn, Cr, V and C at the Σ5(310)[001]36.9° STGB and for selected cases, Σ3(112)[1$\bar{1}$0] STGB in α-Fe was investigated by performing spin polarized DFT calculations with respect to a varying number of alloying elements and H atoms at different segregation sites of the GBs. The impact of co-segregation of Mn-C-H, Cr-C-H, V-C-H on GB energy, work of separation and theoretical strength has been studied. Uni-axial tensile tests were performed perpendicular to the GB and theoretical strength was determined from energy-displacement data fitted using the universal binding energy relationship. The thermodynamic model of Rice and Wang was used to determine the (cohesion enhancing or weakening) nature of the segregated elements. Based on our results, we discuss the alloying strategy to prevent H embrittlement of GBs.