MM 9: Interfaces II: Segregation and embrittlement

Time: Monday 11:45–12:45 Location: H39

MM 9.1 Mon 11:45 H39

Multiscale modelling of gallium induced embrittlement in aluminium — •Venkata Sai Pavan Kumar Bhogireddy[1], Mira Todorova[1], Robert Spatschek[1,2], and Jörg Neugebauer[1] — [1]Max Planck Institut für Eisenforschung, Düsseldorf, Germany — [2]Research Center Jülich, Jülich, Germany

Liquid metal embrittlement is a degradation phenomenon in which a solid metal undergoes brittle failure when it is stressed while in contact with a liquid metal. The transition from ductile to brittle metal failure manifests itself by rapid crack propagation which reduces the elongation to failure ratio.

Combining density functional theory calculations with continuum methods, we study the liquid metal embrittlement of aluminium in contact with gallium. Comparing ab-initio calculated energies for a $\Sigma 3$ and a $\Sigma 5$ Al grain boundary and their corresponding surface energies in the presence and absence of Ga, we identify critical Ga concentrations which result in a weakening of the mechanical strength of aluminium.

Parametrising the DFT results in continuum model we obtain the concentration as a function of the strain in the system. In a final step we extend this approach and compute the stress field induced by cracks in bulk and at grain boundaries. The stress field explains the large segregation of gallium atoms at the crack tip and the crack tip's subsequent propagation.

MM 9.2 Mon 12:00 H39

Chemical trends in grain-boundary elasticity from *ab initio* calculations: case study of Σ5(210) Ni_3(Al,Si) — •Martin Friák[1,2], Monika Všianská[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]Montanuniversität Leoben, Leoben, Austria — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We employ quantum-mechanical calculations within the density functional theory to study elastic properties of $\Sigma 5(210)$ grain boundaries (GB) in Ni_3Al with and without segregated Si atoms substituting Al atoms. Anisotropic elastic properties of 64-atom computational supercells (as periodic approximants of GBs) are determined using the stress-strain method. We compare elastic properties of two chemical compositions of the $\Sigma 5(210)$ GB in Ni_3Al with those with Si atoms at different Al positions at this GB. The elastic properties of the $\Sigma 5(210)$ GB Ni_3Al grain boundaries are found to be very different from the bulk (they possess orthorhombic symmetry and are softer) and exhibit high sensitivity to the chemistry of the grain-boundary interface and its surrounding atomic neighborhood. This sensitivity is, nevertheless, limited to only a few atomic layers away from the grain boundary. Comparing our quantum-mechanical results with predictions obtained by linear-elasticity approach we demonstrate deficiencies of the latter and thus a clear need to use *ab initio* methods in this field.

MM 9.3 Mon 12:15 H39

Hydrogen behaviour at structural defects in high-strength steels — •Eunan J. McEniry, Tilmann Hickel, and Jörg Neugebauer — Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The behaviour of hydrogen in high-strength steels is well-known to play a very significant role in the long-term stability and mechanical properties of such materials. Experimental and theoretical work has indicated that structural defects, such as grain boundaries, dislocations, nanovoids and phase boundaries between the matrix and precipitates present in the material, play the most important role in the phenomenon of hydrogen embrittlement.

Using atomistic simulations, we have examined the energetics and diffusion of hydrogen in the vicinity of such extended defects. Particular emphasis has been placed on a wide range of grain boundaries in ferrite, and on semi-coherent interfaces between ferrite and non-metallic inclusions such as TiC and TiN. Due to the large system sizes required to simulate, for example, low-symmetry grain boundaries or misfit dislocations between the matrix and inclusions, conventional ab initio simulations are no longer feasible. In this direction, we have developed scale-bridging atomistic potentials based on the tight-binding approximation, which still allow for a fully quantum-mechanical treatment of the system.

MM 9.4 Mon 12:30 H39

Effect of Sb segregation on conductance and catalytic activity at Pt/Sb-doped SnO2 interface: a synergetic computational and experimental study — Qiang Fu[1,5], Luis César Colmenares Rausseo[2], •Umberto Martinez Pozzoni[3], Paul Inge Dahl[2], Juan Maria García Lastra[1], Per Erik Vullum[2,4], Ingeborg-Helene Svenum[2,4], and Tejs Vegge[1] — [1]Department of Energy Conversion and Storage, Technical University of Denmark, Lyngby, Denmark — [2]SINTEF Materials and Chemistry, Trondheim, Norway — [3]QuantumWise A/S, Copenhagen, Denmark — [4]Deptarment of Physics, Norwegian University of Science and Technology (NTNU)Trondheim, Norway — [5]Current Address: Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

In this work, the effect of Sb segregation on the conductance and catalytic activity at Pt/Antimony doped tin dioxide (ATO) interface was investigated through a combined computational and experimental study. It was found that Sb-dopant atoms prefer to segregate toward the ATO/Pt interface. The deposited Pt catalysts, interestingly, not only promote Sb segregation, but also suppress the occurrence of Sb3+ species, a charge carrier neutralizer at the interface. The conductivity of ATO was found to increase, to a magnitude close to that of activated carbon, with an increment of Sb concentration before reaching a saturation point around 10%, and then decrease, indicating that Sb enrichment at the ATO surface may not always favor an increment of the electric current.