MM 44: Topical Session: Interface-dominated phenomena - Solutes at Interfaces II

Time: Wednesday 17:15–18:30 Location: IFW A

MM 44.1 Wed 17:15 IFW A

Atomic scale analysis on the elemental partitioning across phase boundaries in medium-Mn steels — •Wenwen Song, Yan Ma, and Wolfgang Bleck — Steel Institute (IEHK), RWTH Aachen University

The ultrafine grained medium-Mn steels (3~12 wt.% Mn) emerge as a strong candidate for the 3rd generation of advanced high strength steels, due to its excellent mechanical properties. In the present work, we aim to understand the role of elemental partitioning across the interfaces, in particular the ferrite-austenite phase boundaries, during intercritical annealing and its impact on yielding behaviors. The nanostructured medium-Mn steels were characterized by atom probe tomography (APT), transmission electron microscopy (TEM) and high energy synchrotron x-ray diffraction (SYXRD). The 3D atomic maps show the elements concentration distribution. The elemental partitioning, i.e. C, Mn, Si, as well as the microalloy elements Nb, Mo, across the ferrite-austenite phase boundaries were analyzed. High carbon segregation at the ferrite-austenite phase boundaries were observed after intercritical annealing and air cooling. This segregation resulted in an increase in the yield strength and a pronounced discontinuous yielding phenomenon. The ferrite-austenite interfaces act as preferable nucleation sites for new partial dislocations in austenite and for full dislocations in ferrite. The current study sheds light on novel microstructural design and interface segregation strategies for ultrafine grained multiphase materials through phase-boundary engineering induced strengthening.

MM 44.2 Wed 17:30 IFW A

A quantum-mechanical study of clean and Cr-segregated antiphase boundaries in Fe_3Al — •Martin Friák, Monika Všianská, and Mojmír Šob — Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

We present a quantum-mechanical study of thermodynamic, structural, elastic, and magnetic properties of selected antiphase boundaries (APBs) in Fe_3Al with the $D0_3$ crystal structure with and without Cr atoms. The computed APBs are sharp (not thermal), and they have {001} crystallographic orientation. They are characterized by a mutual shift of grains by $1/2\langle 100\rangle$, i.e., they affect the next nearest neighbors (APB-NNN type, also called APB-$D0_3$). Regarding clean APBs in Fe_3Al, the studied ones have only a very minor impact on the structural and magnetic properties, including local magnetic moments, and the APB energy is rather low, about 80 mJ/m^2. Interestingly, the studied APBs play a crucial role in the anisotropic (tensorial) elastic properties. The Cr atoms have a strong impact on magnetic properties and a complex influence on the energetics of APBs. The Cr atoms in Fe_3Al exhibit clustering tendencies even in the presence of APBs and cause a transition from a ferromagnetic into a ferrimagnetic state. The impact of Cr atoms on APB energies in Fe_3Al is found to be ambiguous, including reduction, having a negligible influence or increasing APB energies depending on the local atomic configuration of Cr atoms. As similarly contradicting trends were found in experiments, our results can shed a new light on these experimental data (see M. Friák, M. Všianská, M. Šob, Materials 12 (2019) 3954).

MM 44.3 Wed 17:45 IFW A

Ag segregation induced nanofaceting transition of a Cu tilt grain boundary and its impact on plastic deformation mechanisms — •Nicolas J. Peter, Christian H. Liebscher, Christoph Kirchlechner, and Gerhard Dehm — Max-Planck Insitut für Eisenforschung GmbH

We describe the observation of a nanofaceting transition of an asymmetric tilt GB in Cu upon Ag segregation by atomically resolved scanning transmission electron microscopy. The initially flat {110}/{410} boundary was found to dissociate into Ag-lean {230}/{100} asymmetric facet segments and Ag-rich symmetric {210} segments. Thus, a preferential segregation pattern of stable nanosized facets was found. Further, the influence of Ag solute excess concentration on the facet formation was studied by a diffusion couple. It was found that the asymmetric segment remains constant in size, while the symmetric facet segment increases with increasing solute excess. At the diffusion couple's interface a purely symmetric {210} boundary is found. Following the GB, short asymmetric facet segments are introduced and increase their density until a purely asymmetric GB is found close to the non-segregated reference state. Finally, we linked the observed faceting transition to a change in plastic deformation behaviour by tensile straining GB containing bicrystals in situ inside the electron microscope. While pure Cu reference boundaries deform by local emission of partial dislocations resulting in the formation of a single deformation twin, the Ag segregated bicrystal shows numerous partial dislocation nucleation sites resulting in an increase of deformation twins.

MM 44.4 Wed 18:00 IFW A

Influence of impurities on the grain boundary strength in Ir — •Minaam Qamar, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

The present work aims to explore the role of segregated impurities on the grain boundary strength in iridium. Ab initio tensile tests were performed on both pure and impurity-segregated high angle symmetric tilt grain boundaries (GBs) and their cohesive strengths were compared. Two distinct GBs, $\Sigma5(210)[001]$ and $\Sigma11(113)[110]$, were chosen for the study with segregated H and Si atoms. The GBs show a contrasting behavior with respect to trapping sites of the impurity atoms: while the relatively loosely packed $\Sigma5$ GB has multiple low energy trapping sites, the close-packed $\Sigma11$ GB has very few. The behavior of the impurities is also markedly different: Si atoms show a much stronger segregation than H atoms. In addition, a detailed analysis of the migration of an H atom through the GBs found that the arrangement of atoms provides an easy migration path into the GB plane and a high energy barrier for reverse migration, effectively trapping the atom in the GB. However, despite the favorable segregation, neither H nor Si do not seem to significantly affect the cohesive properties of the GBs.

MM 44.5 Wed 18:15 IFW A

Microscopic understanding of Zn diffusion in Fe grain boundaries. — •Michael Geier[2], Martin Panholzer[1], Martin Hoffmann[1], Heiko Groiss[2], Kurt Hingerl[1], and Robert E. Zillich[1] — [1]Johannes Kepler University, Linz, Austria — [2]Christian Doppler Laboratory for Nanoscale Phase Transformations, Center for Surface and Nanoanalytics, Johannes Kepler University, Linz, Austria

Zn coatings are widely used for corrosion protection of steel. However, Zn can lead to a weakening of steel grain boundaries during steel processing at higher temperatures. To investigate this liquid metal embrittlement in the presence of liquid zinc, the diffusing properties of a single Zn atom in Fe grain boundaries were studied using density functional theory which treat the Zn-Fe interactions very accurately. In our approach, we built a simple bcc Fe grain boundary or a dislocation in bcc Fe, and placed a Zn atom within both. With the nudged elastic band method we calculated the energy barrier which the Zn atom has to overcome for moving along the grain boundary or dislocation. Additionally we calculated with transition state theory and random walk theory the diffusion coefficient of the one dimensional diffusion of Zn along the grain boundary. Our results show that the Zn atom diffusion depends strongly on the type of lattice defect, i.e. grain boundary or dislocation. However, it turns out that the difference decreases when approaching melting temperature.