# MM 7: Topical Session Interface-Dominated Phenomena - Segregation and Embrittlement

Time: Wednesday 11:15–12:45 Location: H8

**Invited Talk** MM 7.1 Wed 11:15 H8

**Computational methods for grain boundary segregation in metallic alloys** — •Lorenz Romaner[1], Daniel Scheiber[2], Vsevolod Razumovskiy[2], Oleg Peil[2], Christoph Dösinger[1], and Alexander Reichmann[1] — [1]Department Materials Science, Montanuniversität Leoben, A-8700 Leoben — [2]Materials Center Leoben Forschung GmbH, A 8700 Leoben

Modeling of grain boundary segregation phenomena is an important discipline of integrated computational materials design. Several computational methods, including in particular atomistic, thermokinetic or mechanical models are available to model grain boundary excess and to assess the associated material properties. Segregation energies plays a central role in this connection and large databases are being created to get a comprehensive overview over materials. With the availability of such databases, machine learning approaches can be used to learn the trends in the periodic table and get segregation energies even for alloys for which no data exist at present. We present an investigation on machine learning segregation energies obtained from density functional theory simulations. We will discuss the critical role of feature engineering and analyze different physical parameters including cohesive energies, solution energies, geometry of the segregation site and many more. Furthermore, we show results for a variety of metallic alloys focusing on the class of transition metals and on comparison with experiment. Finally, the challenges of machine learning of segregation energies and grain boundary engineering in general will be discussed.

MM 7.2 Wed 11:45 H8

**Revealing in-plane grain boundary composition features through machine learning from atom probe tomography data** — •Xuyang Zhou[1,2], Ye Wei[1], Markus Kühbach[1,3], Huan Zhao[1], Florian Vogel[4], Reza Darvishi Kamachali[5], Gregory B. Thompson[2], Dierk Raabe[1], and Baptiste Gault[1,6] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Department of Metallurgical & Materials Engineering, The University of Alabama, Tuscaloosa, USA — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]Institute of Advanced Wear & Corrosion Resistant and Functional Materials, Jinan University, Guangzhou, China — [5]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany — [6]Department of Materials, Royal School of Mines, Imperial College London, London, UK

The structures of grain boundaries (GBs) have been investigated in great detail. However, much less is known about their chemical features, owing to the experimental difficulties to probe these features at the atomic length scale inside bulk material specimens. Atom probe tomography (APT) is a tool capable of accomplishing this task, with an ability to quantify chemical characteristics at near-atomic scale. Using APT data sets, we present here a machine-learning-based approach for the automated quantification of chemical features of GBs. This machine-learning-based approach provides quantitative, unbiased, and automated access to GB chemical analyses, serving as an enabling tool for new discoveries related to interface thermodynamics, kinetics, and the associated chemistry-structure-property relations.

MM 7.3 Wed 12:00 H8

**How grain boundary doping affects the mechanical properties in ultra-fine grained tungsten and nanocrystalline tungsten composites** — •Michael Wurmshuber[1], Simon Doppermann[1], Stefan Wurster[2], Severin Jakob[1], Markus Alfreider[1], Klemens Schmuck[1], Rishi Bodlos[3], Lorenz Romaner[1], Verena Maier-Kiener[1], Helmut Clemens[1], and Daniel Kiener[1] — [1]Department Materials Science, Montanuniversität Leoben, Jahnstraße 12, 8700 Leoben, Austria — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, 8700 Leoben, Austria — [3]Materials Center Leoben GmbH, Roseggerstraße 12, 8700 Leoben, Austria

Brittle intercrystalline fracture due to weak grain boundaries is a major problem in both refractory metals as well as nanostructured metals. Naturally, it is therefore also the preferred failure mode in ultra-fine grained tungsten, which is a prime candidate for the divertor material in nuclear fusion. In this work, ultra-fine grained tungsten samples doped with various ab-initio informed elements are fabricated and characterized. A clear improvement of mechanical properties could be observed for samples doped with boron and hafnium. Furthermore, nanocrystalline W-Cu samples were fabricated and doped with the same elements. While boron and hafnium also have a positive effect on the mechanical properties in these samples, the addition of rhenium leads to an even more pronounced improvement, pushing the boundaries set by the strength-ductility paradigm.

MM 7.4 Wed 12:15 H8

**Atomistic Insight into Hydrogen Trapping at MC/BCC-Fe Phase Boundaries: The Role of Local Atomic Environment** — •Boning Zhang[1,2], Jie Su[2], Maoqiu Wang[2], Zhenbao Liu[2], Zhigang Yang[1], Matthias Militzer[3], and Hao Chen[1] — [1]Tsinghua University, Beijing, China — [2]Central Iron and Steel Research Institute, Beijing, China — [3]The University of British Columbia, Vancouver, Canada

A physical understanding of hydrogen trapping at microstructural defects such as grain boundaries (GBs) and phase boundaries (PBs) is vitally important for the design of hydrogen embrittlement (HE) resistant metals. As compared with GBs, the mechanism of hydrogen trapping at PBs is rather unclear due to the complex atomic environment. We perform systematic density functional theory (DFT) calculations to reveal the origin of hydrogen trapping at PBs between body centered cubic (BCC)-Fe and NaCl-type carbides (MCs). We found hydrogen trapping energetics at MC/BCC-Fe PBs depend not only on local volume dilation of the trapping sites, but also on the local atomic environment. An array of descriptors such as lattice strain, geometric volume, and charge density, which have been proven to effectively predict hydrogen trapping at GBs, fail to quantify hydrogen trapping at MC/BCC-Fe PBs. We analyzed the electronic interactions at PBs and found that they are closely related to hydrogen binding energies, and the Bader volume of hydrogen is a universal descriptor for assessing trapping energetics at PBs. This study provides a new insight into hydrogen trapping at microstructural defects.

MM 7.5 Wed 12:30 H8

**Ab initio study of hydrogen segregation and embrittlement at grain boundaries in bcc Fe** — •Abril Azócar Guzmán, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Hydrogen embrittlement is a fundamental problem in materials science that affects structural materials such as steel. Grain boundaries in ferritic microstructures play a dual role in the context of hydrogen embrittlement: they could act as H traps and thus reduce the amount of mobile H in the system. Alternatively, this trapping could promote hydrogen enhanced decohesion (HEDE) at the grain boundaries. Understanding the relationship between strain, hydrogen solubility, and cohesive strength can help elucidate the HEDE mechanism and influence the segregation process. We present the results of *ab initio* studies of the effect of H, as well as C, on Fe at $\Sigma5$ and $\Sigma3$ symmetrical tilt grain boundaries. The calculated results show that the presence of H significantly reduces both the work of separation and the intergranular cohesive strength; these quantities can aid to derive traction-separation laws for cohesive zone models in mesoscale simulations. Additionally, we analyse the solubility of H under mechanical load, which allows us to predict H distribution in microstructures with residual stresses, or under applied load.