MM 6: Interface Controlled Properties, Nanomaterials and Microstructure Design I

Time: Monday 10:15–11:30 Location: C 230

MM 6.1 Mon 10:15 C 230

Learning the influence of chemistry on grain-boundary segregation — •Christoph Dösinger[1], Oleg Peil[2], Daniel Scheiber[2], Vsevolod Razumovskiy[2], and Lorenz Romaner[1] — [1]Montanuniversität Leoben, Department of Materials Science, Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Leoben, Austria

The grain-boundary segregation energy is the central quantity for describing the process of grain-boundary segregation which influences interfacial properties. Usually, to obtain highly accurate values for segregation energies, density functional theory is employed, which incurs high computational costs. This makes it impractical to do a thorough study of segregation to multiple grain-boundaries for a range of solutes. To reduce the number of calculation needed for such a complete description, we apply machine learning methods to density functional theory data. In this talk I will show, how one can train machine learning models that cover the periodic table of elements. By combining element specific features and features of the local atomic structure, these models are able to generalize to different elements and grain-boundaries and accurately predict the segregation energies. The method is tested on a comprehensive data-set of segregation energies in W and then applied in an active learning loop for learning segregation in Cr.

MM 6.2 Mon 10:30 C 230

Grain boundary nanofacets stabilized by facet junction interactions in fcc metals — •Tobias Brink, Lena Langenohl, Swetha Pemma, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

If grain boundary (GB) energies are sufficiently anisotropic, GBs can dissociate into facets to reduce their (free) energy. While mostly splitting of asymmetric GBs into symmetric facets is observed, faceting of symmetric GBs into different symmetric GB planes was also reported (mainly for incoherent Σ3 tilt GBs in fcc). This, in any case, introduces line defects at the facet junctions, which typically present a driving force to grow the facets in order to reduce the total number of junctions and thus the system's energy. Often, facets are micrometer sized and facet growth only arrests for kinetic reasons. So far, energetically stable, finite-sized facets have not been observed, even though theoretical stability conditions have been proposed. Here, we show a case where nanometer-sized facets are indeed stable compared to longer facets in [111] tilt GBs in Cu by atomistic simulation and transmission electron microscopy [1]. This occurs for misorientations that deviate from Σ3 (60°), such as Σ19b (46.8°) and Σ37c (50.6°). In constrast to Σ3, these facet junctions lack a Burgers vector component, which is unusual. Thus, only attractive junction interactions via line forces resulting from the GB excess stress remain, resulting in stable facet lengths of 1–3 nm. Atomistic simulations predict that the same phenomenon also occurs in at least Al and Ag.

[1] Brink, Langenohl, et al., arXiv:2309.07595 [cond-mat.mtrl-sci]

MM 6.3 Mon 10:45 C 230

Segregation of light elements (H, B, C, N, O, P, S) to ferritic iron grain boundaries: A first principles study — •Han Lin Mai[1], Tilmann Hickel[1,2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany

Segregation of alloying or tramp elements to grain boundaries can drastically affect the properties of metallic alloys. Understanding segregation to grain boundaries is an important step towards constructing their defect phase diagrams and therefore critical to enable rational grain boundary engineering for alloys design. Smaller elements such as (H, B, C, N, O, P, S) often play a crucial role in segregation phenomena, but their positioning at grain boundaries are often ambiguous and make them challenging to study. To study the large number of possible relevant defect-solute interactions we have performed high-throughput ab initio calculations using efficient and highly automated workflows using pyiron. The study has been performed across a representative set of coincident-site-lattice (CSL) type tilt GBs. Based on the thus constructed large ab initio data sets we derive and discuss chemical and structural trends observed in the solute segregation behaviour. The features which are most important in evaluating site segregation for small elements are derived and discussed. We also benchmark various interatomic potentials against our DFT data to assess their compatibility with segregation studies.

MM 6.4 Mon 11:00 C 230

Exploring the links between local interface chemistry and mechanics using in situ micromechanical testing — •James P. Best — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany

The mechanisms governing dislocation plasticity and fracture at the smallest scales is critically linked to chemistry, in particular at defects, in dictating material behaviour. This has been demonstrated using in situ electron microscopy testing of, for example, copper and tungsten containing trace impurities at grain boundaries. For the study of recrystallised tungsten, in situ microcantilever testing coupled with atom probe tomography provided insights into the effects of impurity segregation on the toughness by placing the notch directly at grain boundaries. For both as-received material and single-crystalline recrystallised tungsten, plasticity was accumulated before failure through ductile crack tip tearing. In contrast, the toughness at grain boundaries dropped sharply, regardless of grain boundary misorientation or grain orientation. Atom probe analysis of the grain boundaries showed segregation of phosphorous to the recrystallised interfaces. Atomistic simulations of a model Σ7 tungsten grain boundary containing phosphorous confirms a significant embrittlement along the decorated boundary. By elucidating such local chemical effects, we aim to pave the way for the design of materials with enhanced strength and toughness.

MM 6.5 Mon 11:15 C 230

Insights into Microstructure Evolution through Continuum Modeling of Disconnection-Mediated Interface Migration — •Marco Salvalaglio[1], Caihao Qiu[2], Jian Han[2], and David Srolovitz[3] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR, China — [3]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China

Interface migration in microstructures is mediated by the motion of line defects with step and dislocation character, i.e., disconnections. We illustrate a continuum model for arbitrarily curved grain boundaries or heterophase interfaces accounting for disconnections' role in the usual phenomenology of microstructure evolution. We discuss recent model advancements and applications. These include accounting for multi-mode disconnections, namely different step heights for disconnections nucleating on a given grain boundary, and phase field modeling. Numerical results are shown to reproduce molecular dynamics simulations. Implications for interface faceting and change in relative orientations of grains are discussed. Refs: Acta Materialia 227, 117178, (2022); Acta Materialia 227, 117463, (2022); Acta Materialia 251, 118880 (2023).