MM 11: Topical Session: Defects of Defects

Time: Tuesday 10:15–13:00 Location: H10

Topical Talk MM 11.1 Tue 10:15 H10

The role of disconnections in the shear-migration coupling of grain boundaries — •Marc Legros[1], Armin Rajabzadeh[1], Romain Gautier[2], Nicolas Combe[1], and Frédéric Mompiou[1] — [1]CEMES-CNRS, 29 rue Jeanne Marvig, 31055, Toulouse, France — [2]UMET, Université de Lille, Cité scientifique, 59655 Villeneuve d'Ascq

Grain-boundary (GB)-based plasticity is an alternative to classical, dislocation-based deformation. It is supposed to play a significant role in nanocrystalline metals (d<100 nm) for example, that contain a large proportion of GBs but virtually no dislocations. Among all the mechanisms potentially able to generate a permanent (plastic) deformation, the dominant one is the so-called shear-migration coupling. Despite a recent increase in simulations studies, its experimental characterization remains very scarce. Aside from experimental obstacles, the problem is very vast as real grain boundaries possess at least 5 degrees of freedom and contains a potentially infinite number of disconnections, a specific defect that combines step and dislocation characters.

Using both in-situ TEM experiments and molecular dynamic simulations (NEB Nudge Elastic Band), we have shown that shear-migration coupling involves the displacement of these disconnections. As dislocations in the crystal, the properties of these disconnections seem to guide the coupling mechanism of migrating grain boundaries. The overarching question becomes whether we should still consider a given GB as a crystalline defect or a network of its own, which mechanical properties (mobility, shear coupling) are governed by its nature or by its defects?

MM 11.2 Tue 10:45 H10

Atomistic simulation of point defects behavior inside grain boundaries — •Sergei Starikov, Matous Mrovec, and Ralf Drautz — Ruhr University Bochum, ICAMS, 44801 Bochum, Germany

The properties of point defects play a key role in the description of many phenomena within grain boundaries (GBs), such as pre-melting or atomic diffusion. Compared to the bulk, point defects inside GB are characterized by low formation energy and high complexity. Thus, the thermodynamic/kinetic properties of GBs strongly depend on the behavior of point defects. To reveal general aspects of this relationship, we studied behavior of vacancies and self-interstitial atoms inside tilt grain boundaries for several metals (Ni, Al, Fe, Nb, Mo and W) using atomistic modeling. The simulations revealed that the self-diffusion along the tilt GBs at low/moderate temperatures is mostly driven by migration of self-interstitial atoms. However, heating leads to a change in the GB diffusion mechanism to a more complex exchange process, not related to specific defects, but similar to atomic diffusion in a liquid. This change is due to the disordering complexion transition of GBs, which also significantly affects GB mobility.

MM 11.3 Tue 11:00 H10

Impact of grain boundary defects on grain boundary diffusion and segregation of Cr in Ni bicrystal — Shraddha Sevlikar[1], Mohan G. Muralikrishna[1], Daniel Gaertner[1], Sergei Starikov[2], Tobias Brink[3], Daniel Scheiber[4], Daria Smirnova[3], Daniel Irmer[5], Bengü Tas[1], Vladimir A. Esin[5,6], Vsevolod I. Razumovskiy[4], Christian H. Liebscher[3,7], Gerhard Wilde[1], and •Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]ICAMS, RU Bochum, Germany — [3]MPI for Sustainable Materials, Düsseldorf, Germany — [4]Materials Center Leoben Forschung GmbH, Leoben, Austria — [5]Mines Paris, PSL University, Évry, France — [6]Université de Lorraine, CNRS, Nancy, France — [7]RC FEMS, RU Bochum, Germany

Grain boundary diffusion of Cr in a near Sigma-11 Ni bicrystal is measured using the radiotracer technique. Opposite to expectations, two distinct contributions to short-circuit diffusion along the nominally single interface are distinguished and related to the existence of two macroscopic facets with distinct inclinations and, as a result, distinct structures. The segregation factor of Cr in Ni is found to be about unity, which is fully supported by ab initio calculations. Using classical atomistic simulations, Ni grain boundary self-diffusion rates are calculated for the symmetric and asymmetric facets. An accelerated self-diffusion kinetics along the asymmetric facet is observed and attributed to the presence of disconnection-like defects. A heterogeneous mechanisms governing atomic migration across distinct facets is corroborated.

15 min. break

Topical Talk MM 11.4 Tue 11:30 H10

Grain Boundary Spinodals: Faceting Instability and the Role of Junction Energetics — •Fadi Abdeljawad — Lehigh University, Bethlehem, PA, USA 18015

Interfaces greatly influence the physical properties and stability of materials microstructures. Of particular interest in crystalline solids are phenomena that occur due to anisotropic interfacial properties. In polycrystalline aggregates, several experimental observations revealed that an initially flat GB profile may facet into hill-and-valley morphologies with well-defined planes and junctions connecting them. Dislocation-like defects exist at facet junctions, which in general connect GB facets with different atomic structures and interfacial properties. Based on classical atomistic simulations and mesoscale modeling, we examine GB faceting transitions and subsequent facet coarsening dynamics. Our modeling framework accounts for anisotropic interfacial energies, and it incorporates junction energetics and their non-local interactions. The hallmark of our approach is the ability to independently examine the various factors affecting this interfacial instability. Theoretical and computational studies predict the dominant growth morphologies as a function of GB facet junction energies. Furthermore, atomistic and mesoscale simulations show that when accounting for junction energetics GB faceting and subsequent facet coarsening is akin to spinodal decomposition in bulk materials. In broad terms, our work provides an avenue to account for GB structural transitions in models of microstructural evolution.

MM 11.5 Tue 12:00 H10

Defect Phase Diagrams for Grain Boundaries in Mg: Chemical trends at Finite Temperatures — •Prince Mathews[1], Rebecca Janisch[2], Tilmann Hickel[1,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum — [3]Federal Institute for Materials Research and Testing (BAM), Berlin

Lattice defects are known to directly influence the behaviour of materials. The framework of defect phase diagrams (DPDs) offers a powerful and knowledge-based approach for the tailored design of materials by controlling defect phases in competition to bulk phases. Using ab-initio methods and automized workflows, the DPD for the example of Ga segregation to Σ7 [0001] 21.78° (sym. plane 12-30) Mg grain boundary is calculated. It predicts a series of defect phase transformations, which turn out to be in good agreement with transmission electron microscopy experiments. Similar to bulk phases, the stabilities of defect phases can change with temperature. Therefore, different approaches to extend the DPD considering the relevant entropy contributions are discussed. A new sub-lattice model, which is focused on the statistics of grain boundary site column coverages, provides promising insights into temperature-dependent processes of defect phase transformations.

MM 11.6 Tue 12:15 H10

A computationally highly efficient analytical model for the description of defect phase diagrams — •Jing Yang, Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Düsseldorf, D-40237, Germany

In this work, we propose an analytical thermodynamic model for constructing defect and surface phase diagrams. The model is capable of accurately describing the composition-temperature dependence of phase transitions on the surface, including order-disorder ones. It provides a promising alternative to the sublattice model, which is commonly used in the CALPHAD framework to describe solution phases with ordering, as we demonstrate using the system of Mg surface with Ca substitutions. First, as a foundational reference we construct the surface phase transition with grand-canonical Monte Carlo simulation coupled with cluster expansion. The system undergoes a transition from a solid solution (disordered) phase at high temperature, Ca-poor condition to an ordered defect phase with 1/3 Ca coverage. We then show that it is possible to accurately reproduce the critical transition

condition with an analytical model assuming a Boltzmann distribution of the phase fractions. Finally, we compare our method with the sublattice model. The proposed method provides a computationally highly efficient and easy-to-parametrize analytical model for constructing defect phase diagrams.

Topical Talk MM 11.7 Tue 12:30 H10

Atomistic structure of fcc-fcc interface in pure iron and in nanomultilayers: insight from atommistic modeling — •Helene Zapolsky[1], Gilles Demange[2], Yuri Borges Gomes Lima[3], Anastasiai Titova[4], and Renaud Patte[5] — [1]GPM, UMR 6634 University of Rouen, France — [2]GPM, UMR 6634 University of Rouen, France — [3]GPM, UMR 6634 University of Rouen, France — [4]GPM, UMR 6634 University of Rouen, France — [5]GPM, UMR 6634 University of Rouen, France

Very great interest in the structure of interphase interfaces between fcc and bcc crystals has historically arisen due to their technological importance in steels. These interfaces also play a crucial role in metallic nanomultilayers (NMLs), where the presence of numerous semicoherent interfaces leads to a broad spectrum of novel and remarkable properties. One such system, the Cu/Mo NML, holds promise for thermal management applications due to the combination of copper's excellent thermal conductivity and molybdenum's low coefficient of thermal expansion. In these systems, defects at the fcc/bcc interface have a profound impact the thermal properties of the materials. Recently, the Quasiparticle Approach (QA), based on the phase-field methodology, has emerged as a powerful computational tool for modeling and predicting the atomic-scale structure of various interfaces. In this work, we employ atomistic modeling to examine the detailed structure of the fcc/bcc interface, exploring the relationship between this structure and the mode of interface propagation during displacive phase transformations in pure iron and in Cu/Mo NML.