MM 32: Topical Session: Defect Phases I

Time: Wednesday 15:45–18:30 Location: SCH A 216

Topical Talk MM 32.1 Wed 15:45 SCH A 216

Defect phase diagrams: Concepts, computational approaches and applications — Marvin Poul, Prince Mathews, Ali Tehranchi, Jing Yang, Mira Todorova, Tilmann Hickel, and •Jörg Neugebauer — Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany

Extending the well-known concept of bulk phase diagrams to defects allows to predict the thermodynamically stable defect states at any given temperature and bulk composition. Similar to bulk phase diagrams such diagrams allow to identify processing conditions where defect states with particularly desirable stoichiometries, structures and properties form. These diagrams thus provide an exciting new approach in designing materials. Modern atomistic tools based on density functional theory or machine learning potentials can provide all the necessary information to construct such phase diagrams but face severe conceptual and computational challenges: The description of such defects requires thermodynamically open boundary conditions as well as the inclusion of a large number of structural, chemical and electronic degrees of freedom. In the presentation, key concepts of efficiently sampling the large configuration spaces associated with computing defect states and phase diagrams will be discussed. Examples of how this insight can be used to understand and control grain boundary formation, morphology or improved corrosion resistance will be given.

MM 32.2 Wed 16:15 SCH A 216

Fully Automated Calculation of Defect Phase Diagrams — •Marvin Poul, Erik Bitzek, and Joerg Neugebauer — Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Deutschland

Understanding the thermodynamics of segregation at crystal defects is an important part of successful materials engineering.[1] We present an efficient method that constructs finite temperature Defect Phase Diagrams (DPDs) for binary alloys from fully relaxed molecular calculations using machine learning interatomic potentials (MLIP) without user intervention and implemented it as a pyiron[2] workflow. A major challenge that we had to address is the combinatorially growing number of different segregation configurations at any extended defect. The proposed method is able to efficiently tackle hundreds of thousands to millions of configurations and is based on a fast proxy model. This model is based on the ACE descriptors and avoids having to evaluate a full MLIP. This proxy model together with the MAXVOL active learning algorithm allows to pre-screen which configurations to calculate with the underlying MLIP. We apply the workflow on the example of Al and Ca segregation to Mg grain boundaries.

[1]: Korte-Kerzel, S. et al. (2022) Defect phases: thermodynamics and impact on material properties, International Materials Reviews, 67:1, 89-117

[2]: Janssen, J, et al. "pyiron: An integrated development environment for computational materials science." Computational Materials Science 163 (2019): 24-36.

MM 32.3 Wed 16:30 SCH A 216

Effect of chemical changes on the defect structures in lean rare-earth free ternary Mg alloys — •Wassilios Delis[1], Deborah Neuss[2], Marcus Hans[2], Dierk Raabe[3], Sandra Korte-Kerzel[1], and Stefanie Sandlöbes-Haut[1] — [1]Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Germany — [2]Materials Chemistry, RWTH Aachen University, Germany — [3]Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Mg is a lightweight structural material with a good specific strength. Unfortunately, it lacks sufficient room temperature formability and therefore a wider commercial use of Mg is hindered. The preferred basal slip and strong basal-type texture were found to be the main reasons for the poor room temperature formability. Alloys containing low amounts of Al and Ca showed a highly increased room temperature ductility. Here, TEM and APT measurements and ab initio calculations showed an increased activity of $< c+a >$ dislocation slip. The effects of the alloying elements are yet not fully understood. Further research has been performed to investigate how the changes in chemistry affect the structure of defects such as boundaries and dislocations.

MM 32.4 Wed 16:45 SCH A 216

High-throughput generation of defect phase diagrams: A case study in grain boundary solute segregation analysis in Ni base alloys — •Han Lin Mai, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Understanding segregation to grain boundaries, and eventually their defect phase diagrams, is critical to enable rational grain boundary engineering for alloys design. Here, we discuss the progress and challenges one may face when generating such a database of defect-solute interactions, in the context of studying of grain boundary segregation of solutes and impurities in Ni GBs. To compute the large number of 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 large ab-initio datasets, we extract and analyse the chemical and structural trends observed in the solute segregation behaviour across the periodic table. The features which are most important in evaluating site segregation are presented and discussed.

15 min. break

MM 32.5 Wed 17:15 SCH A 216

Planar defects in intermetallic $Mg_xAl_{2-x}Ca$ Laves phases — •Ali Tehranchi[1], Tilmann Hickel[1,2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Bundesanstalt für Materialforschung und -prüfung (BAM)

The intermetallic Laves phases that are present in Mg-based alloys when adding Ca and Al beyond the solubility limit have a beneficial impact on the mechanical properties of these alloys. For example, Laves phases have been observed to enhance the alloy's creep resistance and to extend their application to higher-temperature domains. However, the mechanism of deformation of these phases and their effect on the surrounding matrix is not fully understood. Laves phases not only contain planar defects but also their motifs are observed in planar defects in Mg. In this work, using the concept of defect phase diagrams, we study hcp-like planar defects in the C36 phase and the thermodynamically stable Laves-type planar defects in Mg-based alloys. We show, that while conventional bulk thermodynamic phase diagrams fail to predict the experimentally observed phases the predictions obtained by the defect phase diagrams match well with the experiments. Defect phase diagrams thus provide a powerful tool to predict and interpret the formation of chemically and structurally complex motives at defects as function of experimentally accessible and controllable parameters such as temperature or alloy composition.

MM 32.6 Wed 17:30 SCH A 216

Oxygen vacancy formation energies at grain boundaries in perovskite-type electro-ceramics — •Cong Tao[1], Daniel Mutter[1], Daniel F. Urban[1,2], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, 79108 Freiburg — [2]Freiburg Materials Research Center (FMF), University of Freiburg, 79104 Freiburg

Oxygen vacancy concentrations are assumed to play a major role in the electric-field assisted grain growth of technologically relevant single crystal perovskite phases. The underlying effect on the atomic scale is the redistribution of cationic and anionic point defects between grain boundaries and bulk phases due to different defect formation energies in the structurally different regions, accompanied by the formation of space charge zones. In this study, we present results of classical atomistic calculations of oxygen vacancy formation energy profiles across supercells containing the symmetric tilt grain boundaries $\Sigma5\,(210)\,[001]$, $\Sigma5\,(310)\,[001]$, and the asymmetric tilt grain boundary $(430)\,||\,(100)$. The electro-ceramic perovskite materials $SrTiO_3$, $BaTiO_3$, and $BaZrO_3$ were systematically analyzed. We discuss the dependence of formation energies and resulting concentration profiles on composition and grain boundary type.

MM 32.7 Wed 17:45 SCH A 216

Temperature-dependent impact of antiphase boundaries on properties of Fe_3Al — •Martin Friák[1,2], Miroslav Černý[2,3], and Mojmír Šob[4,1] — [1]Institute of Physics of Materials, Czech

Academy of Science, Brno, CZ — [2]Central European Institute of Technology (CEITEC), Brno University of Technology, Brno, CZ — [3]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, CZ

We have performed a quantum-mechanical study of the influence of antiphase boundaries (APBs) on the temperature dependence of selected materials properties of Fe_3Al. We show that the studied APBs very strongly affect thermal vibrations of Fe_3Al and reduce the width of the band gap in phonon frequencies. Our results also show that the Fe_3Al with APBs exhibits higher volumetric thermal expansion than the defect-free Fe_3Al. The computed free energy of APBs is found to be strongly temperature-dependent. It is lower than the static-lattice temperature-independent APB energy and the reduction is enhanced by increasing temperature (to 76% at T = 700 K). We have also addressed the discrepancy between the experimental bulk modulus and previous theoretical results obtained for the defect-free Fe_3Al. Due to the presence of APBs, the bulk modulus is reduced from the value of 173 GPa, that corresponds to the defect-free Fe_3Al, to 153 GPa, i.e. very close to the experimental value of 147 GPa (at T = 0 K). For details see Intermetallics 151 (2022) 107746, DOI:10.1016/j.intermet.2022.107746.

Topical Talk MM 32.8 Wed 18:00 SCH A 216

Towards a Rigorous Theory of Grain Boundary Segregation in Polycrystals — •Christopher Schuh — MIT, Department of Materials Science and Engineering, Cambridge, MA USA

Although grain boundary segregation is pervasive across metals and materials, the models used to describe it generally fall short in one of two ways. One class of models is too approximate, using, e.g., a scalar 'average' segregation energy; the other is too detailed, focusing on specific atomic sites in select boundaries. Both approaches fail to capture the complex range of sites in the grain boundary network of polycrystals. This talk will overview a project in our group at MIT that aims to develop a new type of grain boundary segregation theory that bridges this gap: it is designed to be quantitatively accurate at the level of specific grain boundary sites, but simple enough to admit solution with an isotherm that can be analytically represented. The approach is based on the parameterization of segregation spectra: distribution functions of all the key thermodynamic quantities necessary to capture the full physics of segregation in polycrystals. We address the spectra of: segregation sites and their enthalpies, interaction parameters amongst solutes, and vibrational contributions to the segregation free energy. After describing computational methods to determine these spectra, we then address the problem of high-throughput computation of them for many alloy systems using tools of data science.