MM 50: Topical Session: Interface-dominated phenomena - Thermodynamics and Microstructure Evolution

Time: Thursday 10:15–11:30 Location: IFW A

Topical Talk MM 50.1 Thu 10:15 IFW A

A Density-based Model for Grain Boundary Thermodynamics and Kinetics — •Reza Darvishi Kamachali, Lei Wang, and David Jacobson — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

Despite their nonequilibrium nature, grain boundaries can have lasting effects on the alloys microstructure, especially when interacting with solute atoms. In fact, solute segregation to grain boundaries is identified as a tool for microstructure design. To make the most of its potentials, a quantitative understanding of grain boundary segregation is required. We propose here a model for studying phase stability and microstructure evolution at grain boundaries. A continuous density field and its corresponding gradients are considered to derive grain boundary thermodynamic functions based on available bulk thermodynamic data. Grain boundary equilibrium phase diagrams are obtained. Several results on segregation and phase separation in binary and ternary alloy systems will be discussed. Based on the current model, some new aspects of grain boundary kinetics and solute drag will be presented as well. The current density-based model for grain boundaries can be readily applied for studying and design of polycrystalline materials.

References: [1] Kamachali RD. A Model for Grain Boundary Thermodynamics. ArXiv: arXiv:1907.12231. 2019. [2] Kamachali RD, da Silva AK, McEniry E, Ponge D, Gault B, Neugebauer J, Raabe D. Segregation–Assisted Spinodal and Transient Spinodal Phase Separation at Grain Boundaries. arXiv:1905.07970. 2019.

MM 50.2 Thu 10:45 IFW A

Effect of thermally driven phase separation on the (nanoscale) magnetic properties of Fe-Cr — •Vladimir Vojtech[1], Robin Schäublin[1], Severin Küchler[1], Andras Kovacs[2], Rafal Dunin-Borkowski[2], and Jörg Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Peter Grünberg Institute, Forschungszentrum Jülich, Germany

Ferritic steel is one of the most promising candidates for deployment as structural material in future fusion reactors. However, the harsh operation conditions, with high temperatures and neutron irradiation, will degrade these materials. In particular, ferritic steel can undergo phase separation leading to Cr-rich α' precipitation, which hardens and embrittles the alloy and may change its magnetic nature. As technological ferritic steels are complex in microstructure and chemistry, studies on fundamental microstructural mechanisms are usually conducted on Fe*Cr model alloys. In this work, we study the thermally driven decomposition in the Fe*Cr system with Cr amounts ranging from 5 to 40 wt.% and annealed for 50 hours to 3 months at 500 °C. Scanning transmission electron microscopy (TEM) with energy-dispersive X-ray spectrometry was used to chemically map the α' phase, while magnetometry, Lorentz TEM and electron holography were deployed to study its impact on the magnetic properties. We will discuss in detail the observed pronounced effect of the decomposition on the magnetic domain size.

MM 50.3 Thu 11:00 IFW A

Thermodynamics, atomic and electronic structure of pristine and doped wurtzite ZnO(0001) inversion domain boundaries — •Jochen Rohrer and Karsten Albe — Institut für Materialwissenschaft, Fachbereich Materialwissenschaft, Technische Universität Darmstadt, Germany

ZnO bicrystal samples with (0001)||(0001) and $(000\bar{1})|(000\bar{1})$ inversion domain boundaries (IDB) show strong variations in conductivity with respect to strain which is attributed to a modulation of the barrier height of the electric potential [1]. In this contribution, we aim at gaining atomistic insight into this phenomena using electronic-structure calculations coupled to thermodynamic analysis.

In particular, we present a comprehensive study on prisinte and doped IDBs considering a large variety of structurally and chemically different model geometries. Despite the lack of inversion symmetry we compute individual grain boundary excess energies by an appropriate choice of model geometries. These models contain one IDB and additional surfaces whose excess is calculated separately and then subtracted. For thermodynamically favoured systems we then investigate electronic structure and repsonse to applied strain in detail.

[1] P. Keil *et al.*, *Adv. Mater.* **30**, 1705573 (2018).

MM 50.4 Thu 11:15 IFW A

Atomistic modeling of the influence of precipitates on the yield strength in Al-Ni-Zr eutectic alloys — •Daniel Mutter[1], Johannes Preussner[1], Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

Lightweight construction is important to achieve resource efficient design, particularly in the mobility sector to reduce fuel combustion and CO_2 emission. In order to fulfill the weight, stability and safety requirements, the materials for this purpose have to be light and at the same time exhibit high specific yield strengths. Al is the most important element in this context, and the existence of a eutectic point in many binary Al-alloys (such as Al-Si, Al-Ni or Al-Ca) further facilitates production processes and leads to alloys with good mechanical properties. By including small amounts of additional elements to the eutectic composition and cooling the melt below the critical temperature, finely dispersed intermetallic phases can form. Their existence within the Al matrix has a strong influence on the mobility of dislocations and can strengthen the material considerably (precipitation hardening). Here, we present results of atomistic modeling and simulation of underlying effects in the Al-Ni system with Zr additives, such as anti-phase boundary energies or shear moduli mismatches between the matrix (fcc-Al) and the precipitate phase, which was shown to consist of $L1_2$ ordered Al_3Zr. The properties and a possible influence of the phase boundary between matrix and eutectic phase (Al_3Ni) are also discussed.