MM 36: Topical Session Electron Theory V

Time: Thursday 14:00–16:00 Location: IFW A

Topical Talk MM 36.1 Thu 14:00 IFW A

Thermodynamics and Kinetics of Grain Boundary Junctions — •Guenter Gottstein, Luis Barrales, Lasar S. Shvindlerman, and Bingbing Zhao — RWTH Aachen University, Institute of Physical Metallurgy and Metal Physics, 52056 Aachen, Germany

Grain Boundaries in polycrystals are connected by grain boundary junctions, which coordinate the kinetic behavior of grain boundary systems, like migration or segregation. Therefore, grain boundary networks are likely to behave differently from solitary grain boundaries. We show that grain boundary junctions are crystal defects on their own with specific thermodynamic and kinetic properties and that these properties affect microstructural evolution during grain growth. Novel experimental methods will be introduced on how to determine the thermodynamic and kinetic properties of junctions, and theoretical approaches will be proposed how to modify existing theories of polycrystal kinetics to account for junction effects. Finally, computer simulations of grain boundary motion and grain growth will be presented to demonstrate the effect of junctions on kinetics, grain size, and texture.

Topical Talk MM 36.2 Thu 14:30 IFW A

High-performance permanent magnets - significance of thermodynamics, kinetics and microstructure — •Gerhard Schneider and Dagmar Goll — Aalen University, Materials Research Institute, Beethovenstr. 1, 73430 Aalen

High-performance permanent magnets (pms) like NdFeB magnets are based on outstanding intrinsic and extrinsic (microstructural) magnetic properties. Excellent intrinsic properties as high saturation polarization and large magnetic anisotropy are achieved by combining transition-metal atoms and rare-earth atoms. For outstanding extrinsic properties ideally μm- or nm-scaled textured hard magnetic grains of ellipsoidal shape are required separated by a nonmagnetic grain boundary phase from each other. However, in NdFeB sintered pms deviations ("structural defects") from this ideal microstructure occur due to the chosen alloy composition in the phase diagram (including additives), powder processing, sintering and annealing conditions. As a consequence the microstructure is characterized by hard magnetic grains of polyhedral shape which are completely or partly surrounded by grain boundary phases (metastable magnetic phases, nonmagnetic phases (η-phase, rare earth oxides)) and pores. Especially the metastable phases which crystallize out of a liquid phase at sintering form a complex structure below the eutectic solidification temperature of 650 °C and influence the magnetic properties. The presentation highlights the thermodynamics and kinetics of the grain boundary phases. The systematic quantitative investigation of character and composition of these phases enables a specific tailoring of the properties of high-performance pms.

MM 36.3 Thu 15:00 IFW A

Thermodynamic model of alloy grain boundaries — •Alexander Kirchner — Institut für Werkstoffwissenschaft, Technische Universität, 01062 Dresden, Germany

A facile thermodynamic model for grain boundaries in substitutional alloys is developed. The macroscopic analysis is based on established descriptions of metallic solutions and the universal equation of state at negative pressure. The thermodynamic potential free energy of atoms in grain boundaries is derived as a function of excess volume and composition. Employing Guggenheim's condition for equilibrium between bulk phase and grain boundaries, the interface free energy and segregation enrichment are expressed. For binary systems with known segregation behavior these quantities are calculated. The results show good agreement with experimental data. Despite inherent limitation which are discussed the proposed model is especially useful for the understanding of nanocrystalline materials.

MM 36.4 Thu 15:15 IFW A

Ab initio prediction of thermodynamic data for selected phases of the Al-Mg-Si-Cu system — •Albert Glensk, Blazej Grabowski, Tilmann Hickel, and Joerg Neugebauer — Max-Planck Institut fuer Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237 Duesseldorf, Germany

Al-Mg-Si-Cu alloys are widely used in engineering applications due to their excellent mechanical properties: low density, high hardness and melting temperature. To tailor these properties, quantitative simulations (like CALPHAD) rely on exact thermodynamic potentials which are nowadays mostly derived from calorimetric experiments. First principles calculations emerge as an alternative for reliable thermodynamic functions in cases of non-existent experimental data or in regions of phase boundaries where the reliability of experiments is limited due to the transient nature of metastable phases. We have, therefore, calculated highly accurate ab initio free energies as a function of temperature and molar volume for selected binary, ternary and quaternary phases of the Al-Mg-Si-Cu system with focus on hcp Mg, diamond Si and Mg2Si. Various quantities are derived from the thermodynamic potentials: Gibbs free energies of formation, enthalpies, entropies, heat capacities, thermal expansions, vacancy concentrations etc. We compare our results to a variety of experiments and put special emphasis on temperature effects due to lattice vibrations. We find the Debye model not to be sufficient at high temperatures and demonstrate that our consistent ab initio approach can improve previous CALPHAD parameterizations of Mg2Si with respect to current experiments.

MM 36.5 Thu 15:30 IFW A

Non-scalar cluster expansions for arbitrary configuration dependent observables in advanced materials — •Sascha B. Maisel[1], Nils Schindzielorz[1], Karsten Durst[2], and Stefan Müller[1] — [1]Hamburg University of Technology, Institute of Advanced Ceramics, Denickestrasse 15, 21073 Hamburg, Germany — [2]Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Werkstoffwissenschaften, Martensstrasse 5, 91056 Erlangen, Germany

We use DFT-based approaches to calculate both free energies and various quantities of technological relevance. These include bulk moduli, elastic constants, piezo-response tensors and dielectric constants of high-end materials like Ni-rich alloys and lead-free ferroelectrics. Based on the formalism of the cluster expansion [1] as realized in the UNCLE [2] package, it is possible to expand any configuration dependent observable like the formation enthalpy in terms of its many-body interactions. In this talk, we present several cluster expansions performed for multiple observables simultaneously. These types of cluster expansion each yield the formation enthalpy plus one or more of the aforementioned other quantities. This enables us to relate e.g an elastic constant of a structure with its chemical stability.

[1] J. M. Sanchez, F. Ducastelle, D. Gratias: Physica 128 A, 334, (1984)

[2] D. Lerch, O. Wieckhorst, G. L. W. Hart, R. Forcade, S. Müller: Modelling Simul. Mater. Sci. Eng. 17, 055003, (2009)

MM 36.6 Thu 15:45 IFW A

Temperature dependence of the stacking fault energy in $Fe_{0.716}Cr_{0.200}Ni_{0.084}$ alloy from first principles — •Hojjat Gholizadeh[1,2], Andrei Reyes-Huamantinco[1,2], Andrei Ruban[3], Peter Puschnig[1], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Materials Center Leoben, Austria — [3]Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden

The mechanism of plastic deformation of steels under mechanical stress is governed by the magnitude of the stacking fault energy (SFE). We calculate the SFE for $Fe_{0.716}Cr_{0.200}Ni_{0.084}$ random alloy in paramagnetic austenitic phase in the temperature range 300-1500 K. Our methodology uses the axial interaction (ANNNI) model to calculate the SFE as a function of the free energies of the perfect fcc, hcp, and double-hcp crystal phases. These free energies are dependent on the lattice parameter which is obtained from experimental thermal expansion data, and on the local magnetic moments which are evaluated using DFT calculations and a Monte-Carlo simulation of a magnetic Hamiltonian of independent local moments. The DFT calculations are performed using the exact muffin-tin orbitals (EMTO) method, which enables to use the coherent potential approximation (CPA) and the disordered local moment (DLM) approaches to model the random alloy in paramagnetic state. Our results, in particular the SFE(T=300 K)=15 mJ/m^2 and the hcp↔fcc transition temperature of 550 K, are in good agreement with experiments.