MM 7: Transport - Atoms and Ions II

Time: Monday 11:45–13:00 Location: IFW A

MM 7.1 Mon 11:45 IFW A

Alloys with continuous concentration gradient: comparing experiments with DFT — •Florian Reiter[1], Martin Hoffmann[1], Alberto Marmodoro[2], Andrei Ionut Mardare[1], Cezarina Cela Mardare[1], Saeedeh Sadet Ravandi[1], Achim Walter Hassel[1], and Arthur Ernst[1] — [1]Johannes Kepler Universität, Linz, Austria — [2]Ludwig-Maximilians-Universität München

Numerical methods allow quasi continuous variation of concentration changes in solid solutions via, e.g., the coherent potential approximation in the multiple scattering theory, which is uncommon in experimental methods. By physical vapor deposition it is possible to create compositional libraries of alloy systems, which allows a comparison with continuous experimental results. For this purpose, the resistivity of an Ag-Pd alloy was measured and related with the calculated Fermi surface. The latter can be obtained from the Bloch spectral function evaluated at the Fermi energy. The calculated Fermi surface shows a significant conformance with the expected nonlinear changes in the experimental resistivity data and can hence be considered representative for the electronic structure of the Ag-Pd alloy. In addition, the experimental results agreed qualitatively with the resistivity data obtained from theoretical calculations.

MM 7.2 Mon 12:00 IFW A

Influence of high current densities on nanocrystalline FeC thin films — •Thomas Brede, Reiner Kirchheim, and Cynthia Volkert — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The goal of our study is to understand the influence of high direct current densities on nanocrystalline materials with solute atoms. The latter will be moved by electromigration and causes changes in the microstructure of the host lattice which were in this way the first time described this year [1]. The FeC thin film model system allows to reach current densities up to several MA/cm^2. Different SEM and X-ray techniques are used to observe the changes in microstructure and texture due to the treatment. We will provide detailed experimental results for is model system as well as a mechanism which might explain the observations.

[1] Brede, T., Kirchheim, R., Volkert, C. A. (2020). Anisotropic grain growth in iron-carbon films at high electric current densities. Scripta Materialia, 178, 18-23.

MM 7.3 Mon 12:15 IFW A

Anharmonic self-diffusion coefficients using the finite temperature string method — •Raynol Dsouza[1], Liam Huber[1], Blazej Grabowski[1,2], and Jörg Neugebauer[1] — [1]Max Planck Institut für Eisenforschung, Düsseldorf — [2]Department of Materials Design, Institute of Materials Science, University of Stuttgart

Simulating self-diffusion in solids using molecular dynamics (MD) usually requires high temperatures, where diffusion can occur at a high enough rate. Finite temperature effects can be well represented at low temperatures using phonon calculations in the well-known quasi-harmonic approximation (QHA). However, anharmonic effects that appear well below room temperature, even for a relatively simple thermodynamic property like vacancy formation, are not captured by QHA [1].

In this work, we apply the finite temperature string (FTS) method [2] in combination with thermodynamic integration [3] to obtain self-diffusion coefficients that capture anharmonic behavior. Using this technique, diffusion at temperatures above the threshold at which QHA begins to lose validity, as well as temperatures at which calculations by direct MD are feasible can be accessed. Performing a careful analysis, we obtain a good agreement between our results and those simulated by MD at high temperatures, which further extend down to low temperatures for FCC and BCC crystal systems.

[1] Glensk et al. Phys Rev X 4 (2014)
[2] Vanden-Eijnden and Venturoli, J Chem Phys 130 (2009)
[3] de Koning et al. Phys Rev B 70 (2004)

MM 7.4 Mon 12:30 IFW A

Atomistic spin-dynamics simulation of self-diffusion in bcc Fe — •Sergei Starikov, Matous Mrovec, and Ralf Drautz — ICAMS, Ruhr-University, Bochum, Germany

We investigate vacancy diffusion and atomic self-diffusion in bcc iron using a combined lattice-dynamics and spin-dynamics simulation. The spin subsystem is simulated by a classical Heisenberg model that takes into account the exchange interaction between pairs of magnetic spins. The interactions between atoms were described by a new interatomic potential developed in this work using the force-matching method. This method enables to reproduce with high fidelity energies, forces and stresses computed at the ab initio level for a fine-tuned set of reference structures. An extended validation of elastic, thermophysical and defect properties has demonstrated a wide range of applicability of the potential. The diffusion simulations reveal a strong dependence of vacancy formation energy on temperature that leads to a non-Arrhenius behaviour of the self-diffusion coefficient. The simulation results are compared with available experimental data.

MM 7.5 Mon 12:45 IFW A

Autonomous Calculation Of Defect Transport Tensors — •Thomas Swinburne[1] and Danny Perez[2] — [1]CNRS, CINaM, Marseille, France — [2]T-1, Los Alamos National Laboratory, USA

Defect diffusion tensors are essential ingredients for mesoscale material models, but current calculation methods typically have unquantified uncertainty and require significant end user involvement. We combine a massively parallel sampling scheme controlled by Bayesian uncertainty quantification[1] with graph isomorphisms to compress the configuration space of isolated defects and automatically assign off-lattice defect displacement vectors to any found transition. We sample in a space irreducible under space group symmetries and derive an exact expression for the diffusion tensor involving only transitions between states irreducible under translation. A quantitative convergence metric is provided using bounds on the relative entropy.

[1] TD Swinburne and D Perez, Self-optimized construction of transition rate matrices from accelerated atomistic simulations with Bayesian uncertainty quantification. Phys. Rev. Materials 2018, 2, 053802