MM 71: Methods in Computational Materials Modelling (methodological aspecst, numerics)

Determination of Defect Properties

Time: Friday 9:30–11:00 Location: TC 006

MM 71.1 Fri 9:30 TC 006

Computing the Absolute Gibbs Free Energy in Atomistic Simulations: Applications to Defects in Solids — Bingqing Cheng and •Michele Ceriotti — Laboratory of Computational Science and Modeling, Institute of Materials, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland

The Gibbs free energy is the fundamental thermodynamic potential underlying the relative stability of different states of matter under constant-pressure conditions. However, computing this quantity from atomic-scale simulations is far from trivial, so the potential energy of a system is often used as a proxy. Here we use a combination of thermodynamic integration methods to accurately evaluate the Gibbs free energies associated with defects in crystals, including the vacancy formation energy in BCC iron, and the stacking fault energy in FCC nickel, iron and cobalt. We quantify the importance of entropic and anharmonic effects in determining the free energies of defects at high temperatures, and show that the potential energy approximation as well as the harmonic approximation may produce inaccurate or even qualitatively wrong results.Our calculations manifest the necessity to employ accurate free energy methods such as thermodynamic integration to estimate the stability of crystallographic defects at high temperatures.

MM 71.2 Fri 9:45 TC 006

First-principles calculations of lattice-vacancy diffusion coefficients via non equilibrium ab initio molecular dynamics — •Igor A. Abrikosov[1,2], Davide G. Sangiovanni[1,3], Davide Gambino[1], and Björn Alling[1,4] — [1]Linköping University, Sweden — [2]National University of Science and Technology "MISIS", Moscow, Russia — [3]Ruhr-Universität Bochum, Germany — [4]Max-Planck-Institut für Eisenforschung GmbH, Germany

We revisit the color-diffusion (CD) algorithm in non equilibrium ab initio molecular dynamics (NE-AIMD) and propose substantially more efficient approach for the estimation of monovacancy jump rates in crystalline solids at temperatures well below melting [1]. Considering bcc Mo between 1000 and 2800 K as a model system, NE-AIMD results show that the colored-atom jump rate increases exponentially with the force intensity F, up to F values far beyond the linear-fitting regime employed previously. At the same time, equilibrium rates extrapolated by NE-AIMD results are in excellent agreement with those of unconstrained dynamics. The gain in computational efficiency increases rapidly with decreasing temperatures and reaches a factor of 4 orders of magnitude at the lowest temperature considered in the present study. Moreover, we demonstrate the applicability of the CD algorithm in simulations of Ti monovacancy jump frequencies in a compound, NaCl-structure titanium nitride (TiN), at temperatures ranging from 2200 to 3000 K [2].

[1] D. G. Sangiovanni, et al., Phys. Rev. B 93, 094305 (2016).
[2] D. Gambino, et al., Phys. Rev. B 96, 104306 (2017).

MM 71.3 Fri 10:00 TC 006

Modelling diffusion in non-dilute Ni-Re alloys: A combined kinetic Monte Carlo and cluster expansion approach — •Maximilian Grabowski, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Deutschland

Ni is a base component in high-temperature superalloys and Re is one of the key ingredients to improve mechanical properties in Ni-based alloys, in particular creep resistance. It is, however, not fully understood how Re affects creep in Ni-based superalloys.

Previous studies showed that in the dilute limit there is almost no effect of Re on the diffusivity of the atoms or the mobility of the vacancies. In this study, we extend our investigation to the non-dilute limit of Re by including Re-Re interactions. This enables us to investigate atomic mobilities and segregation behaviour over the entire composition range.

We use a kinetic Monte Carlo (KMC) approach to simulate diffusion in Ni-Re alloys. The key parameter in the KMC model are the diffusion barriers, which are strongly dependent of the local atomic configuration. To obtain an accurate and fast evaluation of the configuration-dependent diffusion barriers, we combine the KMC model with a cluster expansion (CE) approach. The CE is parametrised using energies from density-functional theory (DFT) calculations for a large number of possible Ni-Re configurations. From the KMC simulations, we then extract diffusion coefficients, evaluate the vacancy mobility as a function of Re concentration.

MM 71.4 Fri 10:15 TC 006

First-principles calculations of field evaporation in atom probe tomography — •Michael Ashton, Arpit Mishra, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40273 Düsseldorf

Atom probe tomography (APT) has developed into a key technique for studying 3D element distribution in complex microstructures at near-atomic resolution. At the heart of the technique is the evaporation of single atoms from a very sharp tip exposed to huge electric fields (10^{11} V/m). However, commonly used geometric reconstruction algorithms fail to take into account any details of the evaporation mechanism, such as differences in evaporation between chemical species or from different sites. To shed light on the factors influencing field evaporation, we study desorption from various sites (ad-atom, steps, kinks) on prototypical metal surfaces (Al, W) by means of density-functional theory calculations. From these calculations, we obtain the field-dependent evaporation barriers, which will be used in subsequent APT simulations. We also find evidence for the roll-over effect at steps, that has been proposed to explain orientational bias in evaporation trajectories.

MM 71.5 Fri 10:30 TC 006

Free Energy of Cu/Ag Heterophase Interfaces — •Marvin Poul, Sebastian Eich, and Guido Schmitz — Universität Stuttgart, Stuttgart, Deutschland

The properties of nanocrystalline materials are influenced by the thermodynamics of their interfaces. In particular we are interested in incoherent heterophase interfaces. Using the Frenkel-Ladd[1] method and the framework of interface thermodynamics developed by Frolov and Mishin[2], we present a Monte Carlo method to compute the free interface energy of incoherent Cu/Ag interfaces. All calculations are performed with the thermodynamically accurate Embed-Atom method potential developed by Williams et al.[3], which is known to reproduce the energies of planar defects very well. In general the procedure should be applicable to arbitrary incoherent interfaces.

[1] Frenkel, D., and Anthony JC L. J. Chem. Phys. 81 (1984): 3188-3193. [2] Frolov, T., and Y. Mishin. Phys. Rev. B 85 (2012): 224107. [3] Williams, P. L., Y. Mishin, and J. C. Hamilton. Model. Simul. Mater. Sci. Eng. 14 (2006): 817.

MM 71.6 Fri 10:45 TC 006

Modeling defects and grain boundaries with the amplitude expansion of the phase field crystal model — •Marco Salvalaglio[1], Rainer Backofen[1], Ken Elder[2], and Axel Voigt[1] — [1]Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, Oakland University, Rochester, 48309 Michigan, USA

The Phase-Field Crystal (PFC) approach describes the dynamics of local atomic probability density on diffusive time scales. It is restricted to relatively small systems as it requires fine spatial discretizations. The Amplitude expansion of the PFC model (APFC) is a coarse-grained approach allowing for tackling larger systems. However, it has limitations on the quantitative description of material properties and on 3D systems. We present the realistic modeling and simulations of grain boundary morphologies between tilted/twisted and strained crystals by means of the APFC model. This is achieved through a Finite Element Method framework with advanced computational features and an extension of the model allowing for the control over the energy of defects, grain boundaries and interfaces. Typical planar and spherical grain boundaries are illustrated for different lattice symmetries, namely triangular/honeycomb in 2D as well as body-centered cubic and face-centered cubic in 3D. Moreover, new results concerning the dynamics of spherical grain boundaries are discussed.