

MM 50: Computational Materials Modelling - Defects & Interfaces I

Time: Thursday 10:15–11:30

Location: H24

MM 50.1 Thu 10:15 H24

Reconciling theory and experiment: Ab initio simulations of point defects up to the melting temperature — ●ALBERT GLENSK, BLAZEJ GRABOWSKI, TILMANN HICKEL, and JOERG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf

Experimental measurements of defect concentrations, enthalpies and entropies can be only performed at high temperatures close to the melting point. In contrast, presently employed $T=0\text{K}$ and quasiharmonic DFT calculations are restricted to low temperatures. To bridge this gap a common approach is the extrapolation of the experimental data to $T=0\text{K}$ assuming that the temperature dependence of the vacancy formation energy follows an Arrhenius behavior, i.e., that the defect entropy is independent on the temperature.

Using a newly developed approach we have been able to compute fully ab initio the temperature dependence of the defect formation energy from $T=0\text{K}$ up to the melting point including all relevant free energy contributions, particularly also anharmonic contributions. Our results show a strong temperature dependence of the defect entropy resulting in a hitherto not expected strong non-Arrhenius behavior. Using the explicit temperature dependence we show that the $T=0\text{K}$ extrapolated values reported in the literature are of by a few tenths of an eV for the formation energies and by an order of magnitude in the entropy. It will be shown that the revised energetics have severe consequences when using vacancy energies e.g. as benchmark to design new DFT xc functionals.

MM 50.2 Thu 10:30 H24

Stability and Mobility of Point Defects in Silicon Studied with Hybrid Density-Functional Theory Including van der Waals Interactions — ●WANG GAO and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der MPG, Berlin, Germany

The intrinsic point defects often significantly affect the electronic and optical properties of semiconductors; therefore their study is important from both fundamental and technological points of view. However, our understanding of self-diffusion in Si remains incomplete and full of controversies, despite decades of seminal work on the subject. Here we present a study of the stability and mobility of point defects in Si and heavier semiconductors using hybrid density-functional theory including screened long-range van der Waals (vdW) interactions [1,2]. The reduction in crystal symmetry around defect sites results in pronounced polarization, which strongly depends on the effective dimensionality of the defect. Furthermore, the screened vdW interactions promote the diffusion of interstitials by decreasing the activation energy by as much as 0.5 eV and suppress the formation of vacancies, supporting the self-diffusion mechanism proposed from P mobility experiments [3]. Notably, our calculations explain a series of experimental observations for the diffusion of interstitials, vacancies, and foreign atoms in Si. For heavier and more polarizable semiconductors, such as Ge, GaAs, and InAs, vdW interactions are found to play an increasingly important role on the stability of point defects, increasing the formation energy by as much as 0.27 eV (11.2%). [1] G. X. Zhang, *et al.*, PRL (2011). [2] A. Tkatchenko, *et al.*, PRL (2012). [3] A. Ural, *et al.*, PRL (1999).

MM 50.3 Thu 10:45 H24

Effect of exchange-correlation functionals on vacancy formation energies — ●ROMAN NAZAROV, TILMANN HICKEL, and JOERG NEUGEBAUER — Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany

The key quantity that determines vacancy concentration is the vacancy formation energy. Even small uncertainties in the vacancy formation energy lead to a deviation of the vacancy concentration by several orders of magnitude. In order to analyze the performance of various exchange-correlation functionals (LDA, PBE, PW91, and AM05) in density functional theory, we calculated vacancy formation energies for 12 fcc metals [1]. The obtained results show that generally the calculated vacancy formation energies are lower than the experimental ones. Furthermore, LDA based values are systematically higher, while the PW91 are systematically lower than the PBE vacancy formation energies. A careful analysis of the possible reasons for such results shows that discrepancies between the theoretical result and experiment as well as differences between theoretical values are mainly related to the way the various exchange-correlation functionals describe the internal surface of the vacancy. Based on this insight we propose an improved correction scheme which when postprocessing the DFT results yields a perfect alignment of vacancy formation energies for all exchange-correlation functionals. These corrected values are also in very good agreement with the experimental vacancy formation energies.

[1] R. Nazarov, T. Hickel, and J. Neugebauer, Phys. Rev. B 85, 144118 (2012)

MM 50.4 Thu 11:00 H24

Atomistic modelling of interfaces between cubic and TCP phases in FeCr — ●THOMAS SCHABLITZKI, JUTTA ROGAL, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Stainless steels show a high resistance to corrosion and radiation damage. Those effects are achieved by alloying the steel with high amounts of chromium. At elevated temperatures, however, the formation of topologically close-packed phases, in particular the σ phase is observed in FeCr systems. This σ phase is unwanted, as it increases the brittleness of the material and lowers its corrosion resistance. A first step towards a better understanding of the formation of the σ phase lies in the investigation of interfaces between the bcc and σ phase in FeCr. We employ an adaptive kinetic Monte Carlo approach to study the mobility of Fe and Cr in the different phases and to analyse atomistic processes at the interface that contribute to the transformation between the two phases. These processes can be complex, involve rearrangement of groups of atoms and can be used to form the basis for the development of a kinetic model to study the formation and growth of the σ phase on extended time scales.

MM 50.5 Thu 11:15 H24

Simulation of grain boundary mobilities in Al, Cu and γ -Fe by molecular dynamics — ●FELIX ULOMEK and VOLKER MOHLES — Institut für Metallkunde und Metallphysik, RWTH Aachen

The grain boundary mobility is an important physical property in metals, but its experimental determination is costly. To determine this value by molecular dynamics simulations is still a problem due to various challenges, mainly unsuited molecular dynamics atomic potentials and artificial grain boundary driving forces. We evaluate how these factors influence the migration mechanism of symmetric CSL grain boundaries in Al, Cu and γ -Fe, and calculate their migration velocities. Boundary conditions are kept as similar as possible to have these materials account for different stacking fault energies, and to show its influence on the migration behavior. Further we evaluate the effect of different MD potential types of the same element on the migration behavior and the resulting grain boundary mobility. The different sources for deviations during the simulations are put in relation.