MM 35: Computational Materials Modelling - Phonons & Phase Stability

Time: Wednesday 11:45–13:00 Location: H24

MM 35.1 Wed 11:45 H24

Phonon dispersions in iron: comparing empirical potentials with first-principles calculations and experimental results — •Daniele Dragoni[1], Davide Ceresoli[2], and Nicola Marzari[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Consiglio Nazionale delle Ricerche, Milano, Italy

Many empirical potentials for iron and its alloys are available in literature. Their performance and reliability has been tested for energetics, thermodynamic properties, and relative bcc-fcc stability under martensitic transformation (Bain path). We focus here on phonon dispersions as a robust indicator of potentials' quality. Both the low temperature bcc phase (ferromagnetic α-phase up to 1043 K, and paramagnetic β-phase up to 1184 K) and the higher temperature fcc paramagnetic γ-phase (between 1184 K and 1670 K) are considered and compared to experimental results and, where available, to ab-initio data. This approach provides valuable insight about the relative accuracy of potentials in treating long- and short-wavelength vibrations and elastic constants at different temperatures and for distinct solid phases.

MM 35.2 Wed 12:00 H24

Ab initio finite temperature description of α Ti including anharmonic contributions — •Dominique Korbmacher, Albert Glensk, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Ti and its alloys are technologically relevant for instance for aircraft or medical applications. *Ab initio* methods based on density-functional theory (DFT) are now routinely used to investigate $T=0$ K properties such as, e.g., the influence of alloying elements on titanium's mechanical properties. In contrast, finite temperature DFT studies are rare and, in particular, limited to approximations such as the quasiharmonic model. While the latter is an accurate approximation for many elements, deviations of $\approx 15\%$ are found for the heat capacity of α Ti (hcp) at higher temperatures [1].

In the present study, we investigate the influence of anharmonic excitations on the thermodynamics of α Ti. To overcome long CPU times we use here the recently developed UP-TILD method [2], a coarse graining scheme allowing to reduce the computation time significantly while keeping high accuracy. In the talk we present the contribution of anharmonicity to various thermodynamic quantities of α Ti and discuss its balance with respect to the other finite temperature excitations. Finally, we reveal whether it can account for the observed discrepancy with experiment or whether the problem originates from an inherent shortcoming of the employed DFT functionals.

[1] Z. G. Mei et al., PRB **80**, 104116 (2009).
[2] B. Grabowski et al., PRB **79**, 134106 (2009).

MM 35.3 Wed 12:15 H24

Modelling phonons in Si_xGe_{1-x} alloys — •Ankita Katre, Georg K. H. Madsen, and Ralf Drautz — ICAMS,Ruhr-Universität Bochum, 44780 Bochum, Germany

Si_xGe_{1-x} alloys are important materials both for the electronics industry[1] and for thermoelectric applications at high temperature[2]. Several experimental and theoretical studies report the enhancement of dimensionless figure of merit (zT) of Si_xGe_{1-x} random alloys by reducing thermal conductivity[3,4]. The phonon calculations required to determine the thermal conductivity of random alloys are computa-tionally expensive using DFT. We have therefore developed a model for obtaining phonon spectra of Si_xGe_{1-x} random alloys. The model parameters are extracted from DFT-calculated force constant matrices for pure Si and pure Ge. We include the contributions upto second nearest neighbour as we find that the phonon frequencies obtained by considering only the onsite and first nearest neighbour force constant matrices are not sufficient for approximating the acoustic phonon modes. The model allows us to determine the phonon frequencies for Si_xGe_{1-x} alloys accurately and efficiently without performing *ab initio* calculations.

[1] J. Ouellette, The Industrial Physicist 8, 22 (2002).
[2] G. A. Slack and M. A. Hussain, J. Appl. Phys. 70, 2694 (1991).
[3] H. Lee, D. Vashaee, D. Z. Wang, M. S. Dresselhaus, Z. F. Ren, and G. Chen, J. Appl. Phys. 107, 094308 (2010).
[4] C. Bera, N. Mingo, and S. Volz, Phys. Rev. Lett. 104, 115502 (2010).

MM 35.4 Wed 12:30 H24

Comparison of phonon frequencies and polarization vectors obtained from fitted force constants or from ab initio force constants — •Christian Illg[1], Bernd Meyer[2], and Manfred Fähnle[1] — [1]Max-Planck-Institut für Intelligente Systeme, 70569 Stuttgart, Germany — [2]Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg, 91052 Erlangen, Germany

The calculation of electron-phonon scattering matrix elements is necessary in many physical contexts and requires reliable information about phonon frequencies and polarization vectors. One can calculate the phonon frequencies and polarization vectors from the dynamical matrix which is the Fourier-transformed force-constant matrix. The force constants can either be determined by a fit to experimental data or by an ab initio calculation. It is well known that the fitted force constants cannot be determined unambiguously since the polarization vectors are hard to measure and do not enter the fit [1]. A unitary transformation would alter the force constants while leaving the frequencies unchanged (but the polarization vectors would change). We compare the frequencies and polarization vectors in the whole Brillouin zone obtained from fitted force constants and obtained from ab initio force constants [2]. The results are important to make a statement on the reliability of phonon polarization vectors obtained from fitted force constants.

[1] R. S. Leigh, B. Szigeti, V. K. Tewary, Proc. R. Soc. London, Ser. A 320, 505 (1971)
[2] C. Illg, B. Meyer, M. Fähnle, Phys. Rev. B 86, 174309 (2012)

MM 35.5 Wed 12:45 H24

Atomistic Modelling of Flexoelectricity in Periclase — Philipp Beck, •Johannes Roth, and Hans-Rainer Trebin — ITAP, Universität Stuttgart

We present a molecular dynamics study of flexoelectricity in periclase. Applying a polarizable effective interaction force field, collective flexo-electric response of an inhomogeneously strained periclase sample can be visualized for the first time. The linear response in periclase is verified by simulations. Two of the linear coupling coefficients can be determined as well as the flexoelectric free energy density as a function of strain gradient. We present a first time modelling of flexoelectric domain building. It turns out that domains in periclase are well separated by a wall of Néel-type.