MM 30: Methods in Computational Materials Modelling III: Thermodynamics

Time: Wednesday 10:15–11:45 Location: H 0106

MM 30.1 Wed 10:15 H 0106

Magnetic materials at high temperature from first-principles: disordered magnetism, vibrations, phase stability and magnetic exchange interactions — •Björn Alling — Department of Physics, Chemistry, and Biology, Linköping University, Sweden

First-principles based approaches faces considerable challenges in modeling magnetic materials at high temperature due to the complexity of simultaneously treat the relevant magnetic, vibrational, and structural excitations. Here a first-principles framework is presented capable of calculating thermodynamic and magnetic properties of magnetic materials in their high-temperature paramagnetic state.

Calculations of temperature dependent vibrational spectra, Gibbs free energies and corresponding phase stabilities are based on the disordered local moments-molecular dynamics (DLM-MD) [2,3] The phonon spectra and pressure-temperature dependent phase transition of the hard coating material CrN is derived [5].

Furthermore, the effects of vibrations and structural disorder on the magnetic exchange interactions are derived. We use our approach to calculate the magnetic interactions of amorphous CrN illustrating the effects on magnetism in an extreme case of structural disorder. [6]

[1] B. Alling, T. Marten, and I. A. Abrikosov, Nature Materials 9, 283 (2010) [2] P. Steneteg, B. Alling, and I. A. Abrikosov, PRB 85, 144404 (2012) [3] B. Alling, L. Hultberg, L. Hultman, and I. A. Abrikosov, APL 102, 031910 (2013) [5] N. Shulumba, B. Alling, et al., PRB 89, 174108, (2014) [6] A. Lindmaa, R. Lizaraga, E. Holmström, I. A. Abrikosov, and B. Alling, PRB 88, 054414 (2013)

MM 30.2 Wed 10:30 H 0106

Phonon modes in Binary Crystals with Positional Disorder — •Tadeus Ras and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

Classical DFT relates equilibrium density fluctuations $\delta\rho(\mathbf{q})$ to elastic response [1]. We present the dispersion relations of binary crystals following an approach to crystal elasticity that includes positional disorder [2].

Even a simple Ramakrishnan-Youssouf DFT of binary hard sphere systems predicts a variety of crystalline phases such as disordered fcc [3]. We illustrate the computation of both acoustical and optical phonon eigenfrequencies $\omega(\mathbf{q})$ of these phases in the presence of point defects. Further we point out the link of $\omega(\mathbf{q})$ to mechanical instabilities that may lead to martensitic phase transitions.

$\omega(\mathbf{q})$ can also be derived from the fluctuations $\delta\rho(\mathbf{q})$ itself. We finally refer to a straighforward method of evaluating experimental or simulation positional data.

[1] M. Fuchs, 'Elastic properties of colloidal solids with disorder', Proceedings of the International School 'Enrico Fermi' (2013).
[2] C. Walz and M. Fuchs, Phys. Rev. B, **81** (2010) 134110.
[3] S. W. Rick and A. D. J. Haymet, J. Phys. Chem., **94** (1990) 5212.

MM 30.3 Wed 10:45 H 0106

Sampling of temperature-dependent interactions within the cluster-expansion framework — •Sascha B. Maisel, Albert Glensk, Dominique Korbmacher, Tilmann Hickel, Blazej Grabowksi, and Jörg Neugebauer — Max-Planck Institute for Iron Research, Max-Planck Strasse 1, 40239 Duesseldorf, Germany

Temperature-dependent effective interactions are an enormous improvement over classical n-body Hamiltonians for a variety of reasons. Advantages include a better description of an alloy's remnant solubility in the dilute limit and more accurate predictions at high temperatures, where phonons are non-neglibible. We compare two different methods for sampling such temperature-dependent interaction strengths for the cluster-expansion method. The first method extends upon earlier work by Reith *et al.*, by including quasi-harmonic and electronic excitations contributing to the Gibbs free energy based on density functional theory phonon calculations. The second method samples temperature-dependent effective interactions directly from finite temperature *ab-initio* molecular dynamics simulations. Variations of this sampling procedure can deal with large interatomic relaxations far better than conventional sampling. We discuss the advantages, shortcomings and computational cost of both methods based on preliminary results for the Ni-Ti and Al-Sc systems.

MM 30.4 Wed 11:00 H 0106

***Ab initio* description of unstable phases at finite temperatures: The Ti bcc to ω transition** — •Dominique Korbmacher, Albert Glensk, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Ti-based alloys are a technologically important class of structural materials. A detailed knowledge of their phase diagrams and transitions is important for optimizing the properties of these alloys. However, the occurrence of phases that become thermodynamically and dynamically stable only at high temperatures makes an ab initio computation of phase diagrams a challenging task.

We have therefore developed and applied an *ab initio* based methodology that allows to accurately compute free energies even of unstable phases. The method employs thermodynamic integration starting from a reference of optimized embedded atom potentials that were fitted to reproduce *ab initio* molecular dynamics data for a narrow volume and temperature range. We apply our technique to the bcc phase of pure Ti and compute its free energy up to the melting point. Our results show a second order phase transformation at around 1000 K upon lowering the temperature. A careful investigation of the molecular dynamics trajectories allows us to identify the low temperature phase as the technologically important hexagonal ω structure.

MM 30.5 Wed 11:15 H 0106

First principles study of competing phases in binary Ti-Ta alloys — •tanmoy chakraborty, jutta rogal, and ralf drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

Ti-Ta shows a stable reversible martensitic phase transformation with a transformation temperature well above 350 K. This makes the material relevant for high temperature shape memory alloy (HTSMA) applications. In our study we use density-functional theory (DFT) in combination with the solid-state nudged elastic band (SSNEB) method to analyse the minimum energy paths along the transformation between different phases. From the relative stability of the phases as a function of Ta concentration we estimate trends in transformation temperature. The calculated phonon spectra provide insight into the dynamical stability of the phases and are used to assess thermal properties. Our results predict a range of 20-35 at.% Ta to be most suitable for a stable Ti-Ta based HTSMA.

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