

MM 39: Phase Transitions II

Time: Thursday 12:00–13:00

Location: IFW B

MM 39.1 Thu 12:00 IFW B

Calculation of Phase Diagrams by Monte Carlo Simulation with Lattice Relaxation — ●ROLF ANDERS and FERDINAND HAIDER — Universität Augsburg, Institut für Physik

A method for the calculation of phase diagrams for alloys given by EAM potentials is presented. It is based on a Monte Carlo (MC) simulation in which the type of a single atom is changed in each step. After an accepted MC step the atomic coordinates in the vicinity of the modification are relaxed in order to account for elastic effects.

The phase diagram is determined by running simulations at different temperatures and chemical potentials. The resulting equilibrium concentrations reveal the stable phases, whose structure is then analysed by calculating the radial distribution functions for each kind of pair of atoms.

Results are shown for Fe-Ni and Fe-Cu.

MM 39.2 Thu 12:15 IFW B

Atomistic simulations on polymeric nitrogen — ●JANI KOTAKOSKI and KARSTEN ALBE — Institut für Materialwissenschaft, TU Darmstadt, Germany

Existence of polymeric nitrogen was proposed in 1992 by Mailhot and co-workers [Phys. Rev. B 46, 14419]. Despite significant effort, the structure was synthesized first time a decade later in 2004 by Eremets et al. [Nature Mater. 3, 558]. Interest in this material is due to its enormous energy capacity (more than 140 kJ/mol or 2.0 MJ/g) - 500 times higher than for TNT, for example. This gives promise for applications such as environmentally safe rocket fuel. The material is obtained by applying high pressure and temperature on the conventional molecular nitrogen.

Even though the cubic gauche structure is considered as a school book example of the predictive power of ab initio calculations, it's far from the complete answer for high pressure phases for nitrogen. In fact, within the last few years, more than twenty different new structures have been proposed. We present density functional theory calculations for the free energy of different phases at large temperature and pressure ranges (energy minimization and phonon density of states calculations). Also presented are the thermodynamically most stable (and dynamically stable) phases at intermediate (188-320 GPa) and high pressures (>320 GPa) which were found recently. Further, we have developed an analytic bond order potential (and extended it to non-bond interactions) in order to mimic the experimental setup.

MM 39.3 Thu 12:30 IFW B

A Correction to the Interpolation Functions for phase field

modeling of three or more phases. — ●ABHIK CHOUDHURY¹ and BRITTA NESTLER² — ¹Institute of Computational Engineering, Karlsruhe, Germany — ²Institute of Computational Engineering, Karlsruhe, Germany

The use of the phase field method has spread to the solution of a variety of practical problems, where the usage of a number of phase field parameters becomes necessary. One of the requirements in the phase field methodology is the usage of interpolation functions, for interpolating the energy of the system for all values of the phase fields. The usual interpolation functions for phase field simulations involving two phase field parameters cannot be applied as interpolation functions for the case of multiple phases. The reasons for this are elucidated in this investigation. A correction has been proposed to the interpolation functions that are normally used for the binary phase field models. The results of this correction are shown through simulations. In the phase field model for the present investigation, we use the parabolic multi-obstacle potential term for the surface energy. This is popular because of the ease of calibration to the material properties. However, in the model a symmetric linear third order term is incorporated for changing the shape of the bulk free energy density, to limit the stable solutions to strict binary interfaces. The correlation between the corrected interpolation function and the third order symmetric term is investigated.

MM 39.4 Thu 12:45 IFW B

High-Dimensional Neural Network Potential-Energy Surfaces: From Elemental Solids to Multicomponent Systems — ●JÖRG BEHLER and NONGNUCH ARTRITH — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Recently, artificial Neural Networks (NN) have been shown to provide accurate high-dimensional potential-energy surfaces for condensed systems. The evaluation of these NN potentials is several orders of magnitude faster than the underlying electronic structure calculations, which enables a routine application in molecular dynamics and metadynamics simulations of large systems. However, so far the applicability of the NN potentials has been limited to elemental systems. By combining the flexibility of the NN methodology with physically motivated terms we are now able to include long-range interactions. This is a necessary prerequisite for studying binary systems like oxides and general multicomponent systems with significant charge transfer. The capabilities of the method are demonstrated for zinc oxide as a benchmark system. We show that structural and energetic properties of various phases are in excellent agreement with reference density-functional theory calculations.