MM 28: Intermetallic phases I

Time: Thursday 10:15–11:15 Location: H16

MM 28.1 Thu 10:15 H16

Empirical effective potentials for complex metallic alloys — •Peter Brommer and Franz Gähler — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Complex metallic alloys (CMAs) comprise materials with promising physical properties. Due to the inherent disorder in these systems, the atomic structure is frequently not reliably known in all details. Atomistic computer simulations are an essential tool both for determining the precise atomic structure and for following the microscopic processes responsible for the macroscopic properties. Unfortunately, first-principles simulations cannot cope with the required system sizes and simulated times, and classical effective potentials are rarely available. We present a programme called *potfit*, which determines the parameters of a classical potential by matching it to a large number of reference quantities computed with first-principles methods. These quantities comprise cohesive energies, stresses and forces on individual atoms in a collection of suitable reference systems. Effective potentials for the MgZn, NbCr, CaCd and AlNiCo systems have successfully been constructed and used in molecular dynamics simulations.

MM 28.2 Thu 10:30 H16

On the thermodynamics of the Pt-Rh alloy: Lattice Monte Carlo simulations using a refined BOS mixing model — •Johan Pohl and Karsten Albe — TU Darmstadt, Fachbereich Material- und Geowissenschaften, Petersenstr. 23, D-64287 Darmstadt

The phase diagram of Pt-Rh printed in most collections of phase diagrams shows a broad miscibility gap. Recent theoretical and experimental studies in contrast indicate that this gap does not exist, but that stable low-temperature ordered phases are present. We calculated the critical temperatures of the theoretically predicted ordered structures and short range order at high temperatures by means of Lattice Monte Carlo simulations using a refined BOS mixing model. This model is able to accurately reproduce the enthalpy of mixing at finite temperatures obtained with the cluster expansion formalism and subsequent cluster variation. Given its simplicity, our model allows computationally more efficient Monte Carlo simulations than the cluster expansion and may also be used for the modelling of nanoparticles. We obtained configurational free energies by thermodynamic integration in the semi-grand canonical ensemble for the different solid solution phases and the implications on phase stability will be presented.

MM 28.3 Thu 10:45 H16

Prediction of stable long-period superstructures in Cu-Pd, Ag-Pd and Au-Pd within a first-principles approach — •Stefan Bärthlein[1], Elke Winning[1], Gus Hart[2], Alex Zunger[3], and Stefan Müller[1] — [1]Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602 — [3]National Renewable Energy Laboratory, Golden, Colorado 80401

One- and two-dimensional long-period superstructures (LPS), based on the $L1_2$ substructure, are systematically investigated for the noble metal-palladium alloys Cu-Pd, Ag-Pd and Au-Pd with first-principles methods. Notwithstanding the fact that the experimental phase diagrams of these systems yield totally different features, quite similar behaviour with respect to formation of low temperature ordered LPS-phases (Cu_3Pd: LPS 3 [1], Ag_3Pd: LPS 3, Au_3Pd: LPS 2; {Cu, Au}Pd_3: $L1_2$, $AgPd_3$: not a ground state) is predicted. As a lever between via LDA obtained formation enthalpies and a thorough ground state scan, the cluster expansion method in conjunction with a genetic algorithm [2] provides adequate means for the extraction of effective interactions, which also allow for an enhanced ground state scan in the configurational space of LPS structures. As a result, the sequences and energetical hierarchies for stable LPSs in Cu-Pd, Ag-Pd and Au-Pd are predicted and compared to conclusions based on an ANNNI-approach. (Supported by DFG.)

[1] Stefan Bärthlein et al., J. Phys.: Fast Track Comm., accepted (2006)

[2] Gus L. W. Hart et al., Nature Materials **4** 391 (2005)

MM 28.4 Thu 11:00 H16

An atomistic view on brittle fracture of complex metallic alloys — •Frohmut Rösch and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Cracks in brittle solids propagate by successively breaking bonds. The fracture behaviour on this atomic level can be mimicked and understood with the help of molecular dynamics simulations. For this purpose we investigate the Friauf-Laves phase C15 $NbCr_2$. The effective potentials for this structurally already quite complex alloy have been matched to ab-initio data for the intermetallic compound. The simulation results reveal that the discreteness of matter strongly effects crack propagation. For this reason major aspects of the computer experiments cannot be explained by continuum theories and global fracture criteria.