

MM 33 Symposium Materials Modelling II

Time: Thursday 14:45–16:30

Room: IFW A

Keynote Talk

MM 33.1 Thu 14:45 IFW A

The first coarse-graining step in alloy theory from the electronic to the atomic level: Transferable potentials and cluster-expansion method — ●MANFRED FÄHNLE¹, RALF DRAUTZ^{1,2}, ALESSANDRO DIAZ-ORTIZ¹, FRANK LECHERMANN^{1,3}, REINHARD SINGER¹, and HELMUT DOSCH¹ — ¹MPI Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart — ²Department of Materials, University of Oxford, Oxford, OX1 3PH, UK — ³Ecole Polytechnique, CPHT, Palaiseau, F-91128, France

For the comprehensive description of the properties of alloys and compounds a combination of theories on various scales is required. On the most fundamental scale, i.e., the electronic scale, the density functional electron theory is able to yield reliable information for single systems, but it cannot scan a very large variety of competing structures in order to determine the ground-state structures or the finite-temperature phase diagrams in multi-component systems. To do this, a first coarse-graining step from the electronic to the atomic scale is required. It is shown [1] that this can be achieved, in principle without losing the accuracy of the ab-initio calculations, by means of transferable potentials and by the cluster-expansion method (CE). The recently developed methods to construct terminated but well-converged CEs are discussed, as well as extensions of the CE method to magnetic degrees of freedom. The power and the remaining limitations of the presently established versions of the CE method are demonstrated for a variety of technologically interesting systems.

[1] R. Drautz et al., J. Phys.: Cond. Matter **16**, 3843 (2004).

MM 33.2 Thu 15:15 IFW A

Efficient tools for the surface cluster expansion of binary alloy surfaces — ●OLE WIECKHORST and STEFAN MÜLLER — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen, Germany

The combination of density functional theory (DFT) with concepts from statistical physics is applied to the segregation at binary alloy surfaces. The binary alloy problem is solved in the cluster expansion by mapping DFT-based formation enthalpies of a number of selected input structures onto a finite set of pair and multibody interactions corresponding to characteristic figures like triangles, tetrahedrons, etc. One critical point of this concept is the selection of an appropriate set of figures, especially when the surface comes into play, which can be solved by treating this selection problem with a genetic algorithm. The number of figures, that has to be selected can be reduced dramatically by properly choosing a reference energy, which can be viewed as an approximation to the surface formation energies. It will be shown how the mixed space cluster expansion can be used to incorporate additional relaxation effects at the surface into this reference energy, thus reducing the need for a large number of manybody figures to compensate for large relaxation energies. As an example, we studied antisite segregation [1,2] in the B2-CoAl(100) surface. (supported by DFG)

[1] V. Blum et al., Phys. Rev. Lett. **89**, 266102 (2002).

[2] O. Wieckhorst et al., Phys. Rev. Lett. **92**, 195503 (2004).

MM 33.3 Thu 15:30 IFW A

Ab initio calculation of thermodynamic properties of metals: xc-related error bars and chemical trends — ●BLAZEJ GRABOWSKI, TILMANN HICKEL, SIXTEN BOECK, and JÖRG NEUGEBAUER — Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf

Phase diagrams are indispensable tools in predicting material evolution during its processing. Current approaches to obtain such phase diagrams (e.g. CALPHAD) are based on extra- and interpolation of experimental data. Experimental costs and unreachability of metastable phases needed for these methods necessitate *ab initio* calculations without experimental input.

The accuracy of density-functional based *ab initio* methods is, in principle, only limited by the exchange-correlation functional. We have therefore evaluated the accuracy of the most commonly used functionals (LDA, PBE-GGA) by calculating key thermodynamic properties for a wide range of metallic materials (Fe, Al, Cu, Rh, Li, etc.). In particular, we have calculated the volume dependence of the free energy employing the quasiharmonic approximation. Great care was taken to ensure sufficient convergence with respect to supercell size, k-point sampling, and

energy cutoff. Based on these results, we have derived thermodynamic quantities such as the thermal expansion coefficient and the temperature dependence of the free energy, which yield a direct insight into the quality of LDA and GGA for the various metals when compared to experimental data.

MM 33.4 Thu 15:45 IFW A

First Principles Calculations of the Elastic Constants of Fe-Pt Phases — ●NIKOLAY ZOTOV and ALFRED LUDWIG — Forschungszentrum Caesar, Ludwig-Erhard-Allee 2, D-53175 Bonn

The electronic structure of the ordered and disordered Fe-Pt phases has been extensively studied during the last two decades by ab-initio methods due to their outstanding electronic and magnetic properties. For example, thin films containing the fct ordered FePt phase are promising candidates for high-density recording media. Their elastic properties have received less attention although the bulk modulus anomaly in FePt alloys is experimentally known since long time. We have carried out a first-principles study of all zero-pressure elastic constants for the ordered Fe-Pt alloys including pure bcc Fe and fcc Pt. The calculations were made using the VASP code implementation of the density functional theory in the generalized gradient approximation (GGA) with Perdew-Wang exchange correlation and projector augmented wave pseudopotentials. The integrations of the Brillouin zone were made on a mesh of 11x11x11 k-points. The calculated elastic constants for bcc Fe and fcc Pt are in good agreement with experimental data and previous calculations. Several trends in the predicted elastic constants are established as a function of the chemical composition. The bulk and shear modulus as well as c_{11} , c_{12} and c_{44} have a minimum for the $F_{e3}Pt$ phase and a maximum for the fct FePt phase. The calculated elastic constants obey all conditions for mechanic stability of the cubic and tetragonal phases but $c_{11} - c_{12}$ is close to zero for $F_{e3}Pt$ suggesting a shear instability at this composition.

MM 33.5 Thu 16:00 IFW A

Temperature dependent properties of Ni₂MnGa — ●TILMANN HICKEL, BLAZEJ GRABOWSKI, OLIVER MARQUARDT, and JÖRG NEUGEBAUER — Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

The ferromagnetic shape memory compound Ni₂MnGa undergoes a martensitic phase transition at 200 K. For temperatures well above this value it has a cubic L2₁ structure, whereas below the transition temperature the structure is orthorhombic. The resulting deformations drive the shape-memory effect. In order to understand the microscopic processes connected to this phase transition, we have investigated its temperature dependence combining density functional theory in the generalized gradient approximation and thermodynamic concepts. For this purpose, phonon and magnon spectra have been determined. Employing the quasiharmonic approximation we have calculated free energy surfaces as function of key reaction coordinates (lattice constant, c/a-ratio). A detailed analysis of the temperature dependence of the surface minima and the low energy paths allowed to extract direct information regarding the thermodynamic stability of the different phases (austenite, martensite, pre-martensite) and activation barriers. The results are compared with recent experiments.

MM 33.6 Thu 16:15 IFW A

High-precision mixed-space cluster expansion for Cu-rich Cu-Pd alloys: Controlling the LPS group — ●S. BÄRTHLEIN¹, G.L.W. HART², A. ZUNGER³, and S. MÜLLER¹ — ¹Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — ²Department of Physics and Astronomy, Northern Arizona University, Flagstaff, Arizona 86011-6010 — ³National Renewable Energy Laboratory, Golden, Colorado 80401

A remarkable feature of Cu-Pd alloys is the existence of long-periodic superlattices (LPS) on the Cu-rich side of the phase diagram. Whereas earlier studies did not include necessary information about the diversity of important, but until then inaccessible formation enthalpies, we are able by combining DFT calculations with a mixed-space cluster expansion, genetic algorithms [1] and Monte Carlo to predict the phase stability from millions of possible candidates. Effective interactions were constructed, enabling us to predict and to study the realm of one-dimensional (1D),

two-dimensional (2D) and three-dimensional (3D) LPS with 1D-LPS3 being the $T = 0\text{K}$ ground state at $x_{Pd} = 0.25$. Furthermore, we investigate the so-called “ $L1_2$ ” phase, which emerges as a domain-mixture between the LPS3 and a newly discovered low-temperature phase at $x_{Pd} = 0.125$. Examination of the systems short-range order reveals a continuous transition from the domain-mixture to the disordered solid solution. (Supported by DFG and NSF.)

[1] G.L.W. Hart et al., Nat. Mater. **4**, 391 (2005)