MM 7: Intermetallic Phases I

Time: Monday 10:15–11:15 Location: H5

MM 7.1 Mon 10:15 H5

Effective potentials for Al–Mn–Pd — •Daniel Schopf, Peter Brommer, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

The Ξ-phases of Al–Mn–Pd are approximants of a decagonal quasicrystal with a lattice constant of 1.6 nm in the periodic direction. The unit cell of these phases contains so many atoms that the capabilities of first-principle DFT methods are exceeded by far. In order to study their structure in detail, reliable effective potentials are needed.

We have developed new analytic embedded atom method (EAM) model potentials and determined their parameters by the force-matching method. The analytic expressions are discussed. Tests with several structures will be presented.

In particular potentials for the ξ- and ξ'-phases of Al–Mn–Pd were established. Material parameters like the elastic constants were calculated. The potentials will be used to improve the structure models for the Ξ-phases and the cores of their metadislocations.

MM 7.2 Mon 10:30 H5

No miscibility gap in Pt-Rh bulk alloys — •Sascha Maisel, Tobias Kerscher, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany

The phase diagram of Pt-Rh possesses an fcc-based solid solution that is stable over the whole concentration range for higher temperatures. However, for low temperatures (< 1000 K) a miscibility gap is deduced, merely from experiments on other alloys [1]. Our theoretical study comprises an ab-initio-based cluster-expansion in the framework of the UNCLE code [2]: We use input data from density-functional theory and subsequent Monte-Carlo simulations in order to account for temperature effects. Our results show that the predicted phase-separation does not occur. The resulting phase diagram will be discussed.
Supported by Deutsche Forschungsgemeinschaft

[1] B. Predel, *Landolt-Börnstein, New Series, IV/5a*, Springer 1991
[2] D. Lerch *et al*, Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009)

MM 7.3 Mon 10:45 H5

Ab-initio optimization of the crystal structure ksi and ksi* in Al- Mn-Pd — •Alejandro Santana Bonilla[1,2], Michael Engel[3], Hans-Rainer Trebin[1], and Marek Mihalkovic[4] — [1]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart — [2]Grupo de sistemas complejos, Universidad Antonio Nariño, Bogotá, Colombia — [3]University of Michigan, Ann Arbor, MI, USA — [4]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia

A structural model is given for two approximants, ksi and ksi*, of the decagonal Al-Mn-Pd phase. Both structures were shown to be completely described by two sorts of interpenetrating clusters, namely *Distorted Bergman Cluster* (DBC) and by *Pseudo Mackay Cluster*(PMC). On the basis of these two atomic clusters the two phases can be characterized as some simple periodic tiling of assembly of the column clusters projected onto the plane perpendicular to the 1.6 nm stacking axis. From crystallographic studies the skeleton of heavy atoms was fully described, whereas the inner shell from PMC was poorly detailed. The structural models have been investigated using ab initio and molecular dynamics numerical methods. For this study, suitable improved pair potentials were used in order to determine the ideal cluster structure and the interactions between adjacent clusters. Plausibility of the suggested structures was tested using competing crystalline phases obtained through convex hull calculations and allowing us to suggest a reliable atomic model for the inner shell of the PMC.

MM 7.4 Mon 11:00 H5

Low temperature phases in Ni-rich Ni-W and Ni-Re — •Nils Schindzielorz, Katharina Nowak, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudstr. 7, D-91058 Erlangen

It is known from experiment [1] that the mechanical properties of Ni-based superalloys heavily depend on the individual amount of W and Re in the alloy. To understand this different behaviour a detailed knowledge of the zero Kelvin groundstate diagram would be of great importance. We find, by use of a density functional theory driven cluster expansion performed with the program package UNCLE [2], that the zero Kelvin groundstate diagrams for Ni-Re and Ni-W with all possible structures based on an fcc lattice up to 20 basis atoms differ significantly. While for Ni-Re we find only one groundstate i.e. the D1a structure at 20 at.% Re, for Ni-W there are six stable groundstates with concentrations less than 40 at. % W.
Supported by Deutsche Forschungs-Gemeinschaft.
[1] H.S.Ko et al., J. Mater. Sci. **33** (1998) 3361
[2] D.Lerch et al., Modelling Simul. Mater. Sci. Eng. **17** (2009) 055003 (19pp)