MM 9: Intermetallic Phases I

Time: Monday 14:45–15:45 Location: IFW B

MM 9.1 Mon 14:45 IFW B

Ab-initio based study of antisite-precipitates in B2-CoAl — •Nils Schindzielorz and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudstr. 7 D-91058 Erlangen

It is well-known that for high temperatures around 1500K the B2-phase of CoAl up to about 70% Co is stabilized by the existence of so called antisite atoms [1]. By quenching the crystal to low temperatures, this phase separates into an ideal B2-CoAl crystal and precipitates consisting of Co antisites only. By the combination of a density functional theory based cluster expansion Hamiltonian with Monte-Carlo simulations it will be demonstrated that these Co clusters show a characteristic size-shape-temperature dependence. Furthermore, we find a flattening of the precipitates at low temperatures due to the anisotropy of the interfacial energy which is wiped out at higher temperature by entropy. A detailed knowledge of the structure of these nanoclusters is of special importance as they lead to local magnetism in a non-magnetic intermetallic compound.

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

MM 9.2 Mon 15:00 IFW B

Effective potentials for rhenium in Ni–Al superalloys — •Peter Brommer[1,2], Stefano Angioletti-Uberti[2], and Mike Finnis[2] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Thomas Young Centre, Imperial College, London, UK

It is widely believed that rhenium, which is commonly used in alloys for turbine blades, is important in increasing the creep resistance of nickel-based superalloys, but the exact reason for this so-called "rhenium-effect" remains unclear.

Atomistic simulations could help study the influence of rhenium on the mechanical properties and compare it to that of other alloying elements. These simulations require effective interaction potentials, as only with those the required large number of particles can be studied. We generated rhenium interaction potentials with the force matching method, where the parameters of a potential are adjusted to optimally reproduce the forces, energies and stresses in a number of reference configurations, which have been evaluated with first-principles density functional theory (DFT) methods.

We use these potentials to study self-diffusion coefficients in liquid and solid alloy phases and compare the results to ab-initio data.

MM 9.3 Mon 15:15 IFW B

Structural stability of topologically close-packed phases in transition metals — •Thomas Hammerschmidt[1], Bernhard Seiser[2], Ralf Drautz[1], and David G. Pettifor[2] — [1]ICAMS, Ruhr-University Bochum, Bochum, Germany — [2]Department of Materials, University of Oxford, Oxford, UK

The formation of topologically close-packed (tcp) phases in Ni-based superalloys leads to the degradation of the creep properties of the alloys. The precipitation of the tcp phases is attributed to refractory elements that are added in low concentration to improve creep resistance. We have compiled a structure map of the occurrence of tcp phases in binary transition metal (TM) compounds. The structure map displays well-established structural trends that are driven by the d-band filling. It also shows that different sizes of the elements tend to stabilize the Laves phases over other tcp phases. The same trend is reproduced in our extensive density functional theory (DFT) calculations of the tcp phases A15, C14, C15, C36, μ, σ, and χ. We show that the structural trend can be understood using the canonical d-band tight-binding model. The small positive values of the heats of formation of all tcp phases suggest that entropy plays a key role in the stabilization of the experimentally observed tcp phases in TM binary compounds.

MM 9.4 Mon 15:30 IFW B

Structural trends in topologically close-packed phases — •Bernhard Seiser[1], Thomas Hammerschmidt[2], Ralf Drautz[2], and David Pettifor[1] — [1]Department of Materials, University of Oxford, Oxford, UK — [2]ICAMS, Ruhr-University Bochum, Bochum, Germany

The creep properties of modern single-crystal Nickel-base superalloys are improved by adding refractory elements. This route of material design is limited by the precipitation of topologically close-packed (tcp) phases which can lead to failure during service. We have assessed the modelling techniques PHACOMP and CALPHAD which are commonly used to predict the tendency of tcp phase formation in austenitic alloys. Moreover, within a tight-binding framework, we have derived analytic bond-order potentials (BOP) that depend explicitly on the valence of the transition metal elements. In particular, we applied these BOPs to investigate the structural stability of tcp phases with respect to the filling of the d-band. From these BOP calculations, we find two groups of tcp phases that exhibit very similar dependence on the d-band filling: A15 and σ on one hand and μ and the Laves phases C14, C15, C36 on the other hand. Through the BOPs we have been able to unravel the link between structural stability and local topology and have identified the interactions that favour the formation of tcp phases.