MM 37: Computational Materials Modelling V - Point defects

Time: Wednesday 10:15–11:15 Location: IFW D

MM 37.1 Wed 10:15 IFW D

Solute-vacancy interaction and diffusion of selected elements in Ni-based superalloys. — •Sergej Schuwalow, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

The dependence of high-temperature properties of Ni-based superalloys on the alloying additives is a subject of ongoing research. Current knowledge is mostly phenomenological in nature and the details of solute diffusion, interaction with defects such as interfaces, vacancies, and dislocations as well as the interplay between composition and microstructure are not well understood.

In this work we investigate the solute-vacancy interactions and concentration/temperature-dependent diffusion behavior of selected alloying elements using a combination of density-functional theory calculations and kinetic Monte Carlo simulations.

Vacancy mobility is found to be only weakly influenced by solute presence, even for heavy refractory elements such as Re. Diffusion coefficients calculated by our approach are shown to be in good agreement with both experiment and simpler, but more limited, analytic models.

MM 37.2 Wed 10:30 IFW D

Effect of Fe and Cu doping on properties of TiNi Alloys — •Martin Zelený[1,2], Xiangqian Yin[2], and Xujun Mi[2] — [1]Institute of Materials Science and Engineering, NETME Centre, Brno University of Technology, Brno, Czech Republic — [2]General Research Institute for Nonferrous Metals, Beijing, P. R. China

The effect of Fe and Cu on the martensitic transformation behavior and mechanical properties of TiNi alloys has been investigated by calculating of the lattice constants and elastic moduli of the B2 phase. The site preference for both doping elements has been studied as well. The calculations were performed using the coherent potential approximation implemented within the framework of the exact muffin-tin orbitals method. Our theoretical results show contraction of the lattice constant of TiNi with increasing concentration of Fe. Added Fe atoms will always occupy the Ni sublattice even in the alloys where Ti is in deficiency. On the other hand added Cu atoms will occupy the sublattice of element in deficiency. This result has been also confirmed by our XRD measurements.

The calculated elastic constants allow us to predict the martensitic transformation temperature, because this temperature is correlated with the C_{44} elastic constant. The composition dependence of elastic moduli and stability of B2 structure is discussed on the basis of the electronic density of states and phonon density of states.

MM 37.3 Wed 10:45 IFW D

Sublattice solubility of transition metals in $L1_2$ phases in Co-based superalloys — •Jörg Kossmann[1], Thomas Hammerschmidt[1], Sascha Maisel[2], Stefan Müller[2], and Ralf Drautz[1] — [1]ICAMS, Ruhr-University Bochum, Bochum, Germany — [2]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

Superalloys are a class of advanced materials that are used e.g. to cast turbine blades for aircraft engines because of their good mechanical stability even at high temperatures. They owe their high-temperature toughness to hardening by precipitation of γ' particles ($L1_2$ structure) which coexist with the coherent γ phase (disordered fcc). Since Sato *et al.* first observed a $L1_2$ phase in the ternary Co-Al-W system, Co-based materials have been shown to be promising candidates for the next generation of superalloys. We investigate the solubility of the transitions metals (TM) W, Mo, Cr, Ti, and Ta in $L1_2$-$Co_3(Al_x,TM_{1-x})$ with density functional theory calculations. For the description of the sublattice disorder we use the cluster expansion and special quasi-random structures. This work is part of the collaborative research center SFB/TR 103.

MM 37.4 Wed 11:00 IFW D

Vacancies in fcc metals — •Mostafa Mortazavifar and Martin Oettel — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Tübingen, Germany

Through a cluster expansion of the crystal partition function, we derive an approximate expression for the equilibrium concentration of thermal vacancies in solids which allows for a transparent interpretation of the vacancy volume and the energetic/entropic part in the corresponding Gibbs energy of vacancy formation ΔG_v. For the text–book model crystals made of hard spheres and Lennard–Jones particles very good agreement with simulation data is found. Application to Ni through the embedded–atom method (EAM) reveals a strong sensitivity of the variation of ΔG_v with temperature to details of the EAM potential [1]. We propose to use our formula for $\Delta G_\mathrm{v}(T)$ in reference calculations where the needed partition function terms should be evaluated by quantum density functional theory (qDFT). The results can be employed in theoretical materials science using ab-initio methods or in constructing effective classical potentials.

[1] M. Mortazavifar and M. Oettel, *Thermal vacancies in close–packing solids*, arXiv:1311.5093 [cond-mat.soft]