MM 22: Computational Materials Modelling - Phase Stability II

Time: Tuesday 11:45–13:00 Location: H24

MM 22.1 Tue 11:45 H24

Stability analysis of complex phases in transition-metal alloys with analytic bond-order potentials — •Thomas Hammerschmidt and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Topologically close-packed (TCP) phases play in important role for precipitate hardening in steels and as detrimental brittle phase in single-crystal superalloys. The structural stability of TCP phases can be attributed to an interplay of band-filling effects and differences in atomic size. In order to further understand this interplay, we apply a hierarchy of electronic-structure methods: On the level of density-functional theory (DFT), we determine the formation energies of the TCP phases A15, sigma, chi, mu, C14, C15 and C36 in the binary systems Ta-V/Nb, Re-V/Cr/Nb/Mo, and Co-V/Cr/Nb/Mo. The binary structures as obtained from relaxations by DFT are then analyzed on the basis of a simple canonical tight-binding (TB) model that provides a coarse-grained description of the electronic structure. The solution of the tight-binding problem is computed within the formalism of analytic bond-order potentials (BOPs) as a second coarse-graining step. This enables us to decompose the binding energy in contributions from different neighbor shells in terms of moments of the electronic density-of-states obtained from analytic BOP. We analyze the importance of internal relaxations in the DFT-relaxed structures across the transition metals series for elemental TCP phases. Furthermore we discuss the identification of size effects in binary TCP phases obtained from DFT calculations in terms of moments from analytic BOP.

MM 22.2 Tue 12:00 H24

Structural stability of topologically close-packed phases in the Fe-Nb system — •Alvin Noe Ladines, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Germany

The amount of refractory metals in powder metal steels is limited by carbide formation during atomization of the powder. Diffusion alloying makes it possible to push this limit by starting from a carbon-free melt. This route leads to the formation of topologically close-packed (TCP) phases which are transformed into carbides by subsequent addition of graphitic carbon during powder consolidation. In order to optimize this new processing method, one has to determine the properties of the observed TCP phases and to understand the mechanism of TCP-carbide transformation. In this study, we employ density functional theory (DFT) to determine the stability of TCP phases in the Fe-Nb system. The TCP phases that we considered include the A15, Laves(C14,C15 and C36), χ, μ and σ. Each of the Wyckoff positions were filled with either Fe or Nb allowing us to change the composition of the binary system. According to our calculated values of the heat of formation, the Laves phases and the μ phase are stable with stoichiometric compositions of Fe_2Nb and Fe_7Nb_6, respectively. For the Laves phases we observe a very close competition with the heats of formation differing only by a few meV. Our calculations also suggest a broad stability range for the μ phase extending up to approximately 54 at % Nb. Our findings are consistent with the experimental phase diagram of the Fe-Nb system. In addition, we also determined the influence of C defects on the stability of the Laves and the μ phases.

MM 22.3 Tue 12:15 H24

A cluster-expansion Hamiltonian for the modeling of phase stabilities in the Ni-rich Ni-Al alloy — •Sascha B. Maisel, Michaela Höfler, and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Denickstrasse 15, Building K, 21073 Hamburg, Germany

Binary NiAl forms a well known stoichiometric phase called the γ'-Phase at 25 at. % Al. This phases shows a pronounced $L1_2$ ordering tendency and its precipitates are popular hardeners in many advanced alloys. Effective cluster-expansion interactions for the binary NiAl system between 0 and 25 at. % Al are needed as part of a larger project, which ultimately aims to supply model-Hamiltonians for multicomponent Ni-based super alloys. We have parametrized such an effective Hamiltonian for the Ni-rich Ni-Al alloy and present it in this talk, along with benchmarks of its efficiency and its accuracy in predicting formation enthalpies and phase boundaries when compared to both DFT input and experiments.

MM 22.4 Tue 12:30 H24

Ab-initio study of kappa-carbide precipitates in an austenitic Fe matrix — •Poulumi Dey, Roman Nazarov, Martin Friak, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

The quaternary system Fe-Mn-Al-C exhibits interesting physical properties and is highly relevant for a new class of steels with high strength and toughness. Depending on the composition, experiments show the precipitation of kappa-carbides, (Fe,Mn)3AlC in these steels, which significantly influence the microstructure. In order to theoretically predict the formation of these precipitates, we perform a thorough investigation of the structure, composition and magnetism of kappa-carbides in an austenitic Fe-based matrix with the aid of density functional theory. The formation energy of kappa-carbides is computed as a function of the chemical potentials of its constituents, including the effect of different magnetic structures. For both aspects the constraints posed by an austenitic Fe-Mn-Al matrix have been taken into account. Our results show that the Mn-free Fe3AlC is energetically most favorable over a wide range of chemical potentials and hence most abundant as coherent precipitate in the matrix. An increase in Mn concentration results in a monotonic increase in the lattice constant of kappa-carbides and therefore a growing lattice mismatch between the kappa-carbide and the matrix. The results can be used to design strategies to adjust the amount of kappa-carbides in Fe-Mn-Al steels.

MM 22.5 Tue 12:45 H24

Comparison of Analytic and Numerical Bond-Order Potentials for bcc Refractory Metals — •Miroslav Cak, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

A systematic coarse-graining of the electronic structure leads from DFT to tight-binding and to bond-order potentials (BOP). The calculation of the total energy of a system of interacting atoms can be carried out within the formalism of either analytic or numerical BOP. Recently, we developed parameterizations of analytic BOPs for the refractory metals Tungsten, Molybdenum, Niobium and Tantalum. These refractory metals play an important role as strengtheners of nickel- and cobalt-based superalloys. Here we employ our new parameterizations in a detailed comparison of numerical and analytic BOP and find very good agreement for various bonding configurations. Comparing these BOP calculations to corresponding first-principles, tight-binding and experimental results confirms the transferability of both BOP schemes to atomic structures encountered in lattice defects. As an application of our BOPs we determine the interaction of dislocations with other defects like vacancies.