MM 33: Structural Materials I: Phase Stability and Mechanical Properties

Time: Wednesday 10:15–11:30 Location: TC 010

MM 33.1 Wed 10:15 TC 010

Comparison of Co-X and Ni-X systems with density functional theory and bond-order potentials — •Jörg Kossmann, Alvin Ladines, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Single crystal superalloys are used widely in high-temperature applications. Most of todays superalloys are based on Ni-Al and comprise 10 or more alloying elements. For example, Re and other 5d elements are added to improve creep resistance. Recently, materials based on Co-Al-W where shown to possess a γ/γ' microstrcuture which makes these alloys interesting for singe crystal superalloy applications. We compare and contrast Co-based and Ni-based alloys from high-throughput density-functional theory (DFT) calculations. We relate phase stabilities, lattice constants, and elastic constants in Co-X and Ni-X binaries with X=Al,W,Re and the ternary systems Co-Al-W and Ni-Al-Re. New bond-order potentials (BOPs) are fitted to the DFT results and we obtain satisfactory agreement between BOP and DFT.

MM 33.2 Wed 10:30 TC 010

Analysis of the thermodynamic phase stability in the Al-Sc system using first principles methods — •Ankit Gupta[1], Biswanath Dutta[1], Tilmann Hickel[1], Jörg Neugebauer[1], Yulia Buranova[2], and Sergiy Divinski[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Institute of Materials Physics, University of Münster, D-48149 Münster, Germany

Driven by the need to achieve high strength materials with reduced weight, Al-Sc alloys have received considerable attention in the last couple of decades owing to their superior mechanical and anti-recrystallization behaviour. These improved properties critically depend on Al_3Sc particles that precipitate out from Sc supersaturated solid solution. In experiment, their shape, distribution and morphology show a remarkable variation depending on composition and mechanical load, which has not yet been understood. In this work, we therefore investigate the thermodynamic phase stability of this alloy system within a first-principles based approach with a focus on the Al rich corner of the binary phase diagram. The temperature dependence of the Sc solubility in Al is calculated as an outcome of a competition between the free energies of formation of the dilute solvents and the ordered precipitate phase within the quasi-harmonic approximation. Our results for the thermodynamic and elastic properties of the Al_3Sc phase additionally confirm the experimental finding of coherent precipitates. The investigations are extended towards kinetic Monte-Carlo simulations of the precipitation kinetics in terms of TTT diagrams for the precipitate formation.

MM 33.3 Wed 10:45 TC 010

Correlation between thermodynamic and mechanical properties in Ta-W — •Sandra Hoppe and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

Varying an alloy's concentration or alloying constituents strongly influences its structural and mechanical properties. Modern simulation methods like density functional theory in combination with the cluster expansion make the whole configurational space accessible. This way, also metastable structures may be considered, which are experimentally difficult to obtain. Recent results for several face-centered cubic (fcc) binary metal alloys [1] suggest a linear correlation between thermodynamic stability and elastic properties at a fixed stoichiometry. This study aims to investigate the generality of these findings by considering a similar correlation for binary body-centered cubic (bcc) alloys. As a model system, Ta-W was chosen due to its simple phase diagram with solid solution in the whole concentration range. Interestingly, the elastic constants c_{44} and c_{12} show an opposing trend to that observed for fcc alloys: Energetically favorable structures are mechanically weaker than those further away from the ground-state line. This phenomenon may be related to the anomalous behavior of c_{44} with increasing pressure or temperature, which has been reported in the literature for Ta-W. We will discuss the interesting behavior of Ta-W with regard to its electronic structure.

[1] S. B. Maisel, M. Höfler, and S. Müller. *Nature* **491** (2012) 740.

MM 33.4 Wed 11:00 TC 010

From generalized stacking fault energies to dislocation cores: impact of solutes on the Peierls stress in magnesium — •Zongrui Pei[1,2], Martin Friák[3,1,2], and Jörg Neugebauer[1] — [1]1Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Aachen, Germany — [3]Institute of Physics of Materials of the Academy of Sciences of the Czech Republic, v.v.i, Brno, Czech Republic

Using ab initio calculations and Fourier transform we analyze a basal plane gamma surface in pure Mg and show that the knowledge of energies of only three specific points is sufficient to accurately predict the core structure of <a> dislocations. This finding greatly reduces the computational costs related to the Peierls-Nabarro (PN) model and allows for a high-throughput application of the PN model to dislocation cores in Mg alloys. We employ our approach to study Mg binary alloys containing 9 rare-earth (RE) and 11 other solutes that crystallize in either hexagonal close-packed (hcp) or double hcp (dhcp) structures. Based on the calculated core structures of these 20 Mg alloys, solutes are divided into three groups. The group consisting of Co, Os, Re, Ru, Tc and Ti shows more compact core structures and larger Peierls stress than pure Mg, the group including Be, Hf, Tl, Zn, Zr and Sc (the only RE element in this group) changes both the core widths and Peierls stresses moderately. The third group containing the other RE elements extend the core width from 9b-19b, and the Peierls stresses are generally very low, which shows a solute solution softening trend.

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