MM 2: Topical session: Integrated computational materials engineering for design of new materials I

Time: Monday 10:15–11:45 Location: H38

Topical Talk MM 2.1 Mon 10:15 H38

High-Throughput Computational Search for Precipitation Hardened Alloy Systems — •Chris Wolverton — Dept. of Materials Science and Eng., Northwestern University, Evanston, IL USA 60208

The search for high-strength alloys and precipitation hardened systems has largely been accomplished through Edisonian trial and error experimentation. Here, we present a novel strategy using high-throughput computational approaches to search for promising precipitate/alloy systems. We perform density functional theory (DFT) calculations of an extremely large space of ~200,000 potential compounds in search of effective strengthening precipitates for a variety of different alloy matrices, e.g., Fe, Al, Mg, Ni, Co, and Ti. Our search strategy involves screening phases that are likely to produce coherent precipitates (based on small lattice mismatch) and are composed of relatively common alloying elements. When combined with the Open Quantum Materials Database (OQMD, oqmd.org), we can computationally screen for precipitates that either have a stable two-phase equilibrium with the host matrix, or are likely to precipitate as metastable phases. Our search results produce (for the structure types considered) nearly all currently known high-strength precipitates in a variety of fcc, bcc, and hcp matrices, thus giving us confidence in the strategy. In addition, we predict a number of new, currently-unknown precipitate systems that should be explored experimentally as promising high-strength alloy chemistries.

MM 2.2 Mon 10:45 H38

Facet-controlled phase separation in supersaturated Au-Ni nanoparticles upon shape equilibration — Andreas Herz[1], •Martin Friák[2,3], Diana Rossberg[1], Martina Hentschel[1], Felix Theska[1], Dong Wang[1], David Holec[4], Mojmír Šob[3,2,5], Oldřich Schneeweiss[2], and Peter Schaaf[1] — [1]TU Ilmenau, Ilmenau, Germany — [2]Institute of Physics of Materials, AS CR, Brno, Czech Republic — [3]CEITEC MU, Masaryk University, Brno, Czech Republic — [4]Montanuniversität Leoben, Leoben, Austria — [5]Dept. of Chem., Faculty of Science, Masaryk University, Brno, Czech Republic

Solid-state dewetting is used to fabricate supersaturated, submicron-sized Au-Ni solid solution particles out of thin Au/Ni bilayers by means of a rapid thermal annealing technique. Phase separation in such particles is studied with respect to their equilibrium crystal (or Wulff) shape by subsequent annealing at elevated temperature. It is found that {100} faceting planes of the equilibrated particles are enriched with Ni and {111} faces with Au. Both phases are treated by quantum-mechanical calculations in combination with an error-reduction scheme that was developed to compensate for a missing exchange-correlation potential that would reliably describe both Au and Ni. The observed phase configuration is then related to the minimization of strongly anisotropic elastic energies of Au- and Ni-rich phases and results in a rather unique nanoparticle composite state that is characterized by nearly uniform value of elastic response to epitaxial strains all over the faceted surface. This work demonstrates a route for studying features of physical metallurgy at the mesoscale (APL 107 (2015) 073109).

MM 2.3 Mon 11:00 H38

Heat capacity of the quaternary Q phase in Al-Cu-Mg-Si: a combined ab-initio, phonon and compound energy formalism approach — •Ali Zendegani[1], Fritz Körmann[1], Tilmann Hickel[1], Bengt Hallstedt[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Rheinisch-Westfälische Technische Hochschule Aachen, Aachen, Germany

The Q phase is an important quaternary precipitate in aluminum-based alloys that contain Mg, Si and Cu. These alloys belong to the most promising materials in automotive and aircraft engineering. To tailor their mechanical characteristics via heat treatments, a precise knowledge of their precipitation properties is essential.

In order to achieve an improved thermochemical parameter set of the Q phase, we have performed a combined first-principles, phonon and compound energy formalism approach on this phase to investigate its heat capacity. For a fair comparison with available experimental data, the impact of lattice vibrations on the site occupancy of sublattices has also been taken into account. Excellent agreement with experimental data demonstrates the high predictive power of our first-principles approach [1].

[1] A. Löffler, A. Zendegani, J. Gröbner, M. Hampl, R. Schmid-Fetzer, H. Engelhardt, M. Rettenmayr, F. Körmann, T.Hickel, J. Neugebauer, Journal of Phase Equilibria and Diffusion, in press

MM 2.4 Mon 11:15 H38

Numerical multi-criteria optimization methods for alloy design: Development of new high strength nickel-based superalloys and experimental validation — •Ralf Rettig, Alexander Müller, Nils C. Ritter, and Robert F. Singer — Institute of Science and Technology of Metals, Department of Materials Science and Engineering, University of Erlangen, Martensstr. 5, D-91058 Erlangen, Germany

A new approach for the design of optimum balanced metallic alloys is presented. It is based on a mathematical multi-criteria optimization method which uses different property models to predict the alloy behavior in dependency of composition. These property models are mostly based on computational thermodynamics (CALPHAD-method). The full composition range of the alloying elements can be considered using these models. In alloy design usually several contradicting goals have to be fulfilled. This is handled by the calculation of so-called Pareto-fronts. The aim of our approach is to guide the experimental research towards new alloy compositions that have a high probability of having very good properties. Consequently the number of required test alloys can be massively reduced. The approach will be demonstrated for the computer-aided design of a new Re-free superalloy with nearly identical creep strength as that of Re-containing superalloys. Our starting point for the design was to maintain the good properties of the gamma prime-phase in well-known alloys like CMSX-4 and to maximize the solid solution strengthening of W and Mo. The presented experimental measurements proof the excellent properties.

15 min. coffee break