# MM 35: Topical Session Theory meets Experiment III - Bond-order Potentials and Finite Temperature

Time: Wednesday 15:00–16:15 Location: TC 006

**Topical Talk** MM 35.1 Wed 15:00 TC 006

**Simplified models of the electronic structure for predicting crystal structure stability** — •Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Atomistic simulations may contribute to the theory-aided development of new materials mainly in two ways. Firstly, quantitatively accurate simulations of compound energies and properties may be used to screen materials across compositions and structures. Secondly, qualitative trends in structural stability and other properties may be explained and understood in terms of the bond chemistry and bond formation between the constituents of the material.

In this talk I will give examples for the combination of the two approaches and how they may be of help to suggest new experiments or contribute insight into the behaviour of materials. I will mainly focus on the stability of topologically close-packed phases in superalloys and the magnetic contribution to phase stability in iron and steels.

MM 35.2 Wed 15:30 TC 006

**SAPIENS, a DFT and experimental based thermophysical database for pure elements** — •Mauro Palumbo[1], Suzana G. Fries[1], Thomas Hammerschmidt[1], Ralf Drautz[1], Fritz Körmann[2], Tilmann Hickel[2], and Jörg Neugebauer[2] — [1]ICAMS, RUB, Stiepeler Str. 129, D-44801 Bochum, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany

Steels and Ni-based superalloys are multicomponent and multiphase materials. A theoretical approach for predicting phase stability as a function of composition, temperature and pressure for these materials should use the same method for all the phases since changes in potentials, approximations, etc can introduce differences which are of the same order of magnitude of the differences in energy required to describe the stability of real alloys. We developed a consistent first-principles database for Helmholtz energies from which thermophysical properties such as volume, heat capacity, bulk modulus, thermal expansion, can be calculated. Our approach took into account the contribution of different excitations (phonons, electronic excitations, magnons) for the temperature dependence. The vibrational contribution was evaluated within the Quasi-Harmonic Approximation. The electronic contribution was evaluated using Fermi-Dirac statistics and DFT based electronic Density of State. Magnetism was calculated using Heisemberg hamiltonian and Quantum Montecarlo. The methodology was applied to Fe, Cr, Ni, Al pure elements. Results were compared with an extended set of experimental data.

MM 35.3 Wed 15:45 TC 006

**Bond-order potentials for bcc transition metals** — •Miroslav Cak, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Bond-order potentials (BOPs) are based on the tight-binding approximation for determining the energy of a system of many interacting atoms. We present newly developed parametrisations of analytic BOPs for the refractory metals Tungsten, Molybdenum, Niobium and Tantalum. These metals play an important role as strengtheners of nickel-based superalloys and in topologically close-packed (TCP) phase precipitates in steels. Theory parameters of the analytic BOPs were optimised for the equilibrium bcc structure and extensively tested for atomic environments far from equilibrium that have not been included in the fitting procedure. These tests include structural energy differences for different competing structures; tetragonal, trigonal, hexagonal and orthorhombic deformation paths; formation energies of point defects and phonon dispersion relations. Comparing our calculations to corresponding first-principles, tight-binding and experimental results shows a very good transferability of our analytic BOPs to atomic structures encountered in lattice defects. From phonon densities of states we calculated heat capacities $C_V$ at room temperatures that are in good agreement with experimental values. The new analytic BOPs were also applied to the calculation of melting temperatures using molecular dynamics simulations. Our results are in reasonable agreement with experiment and confirm that our BOPs capture the refractory character of W, Mo, Nb and Ta.

MM 35.4 Wed 16:00 TC 006

**Computing atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron** — •Fritz Körmann[1], Alexey Dick[1], Blazej Grabowski[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany — [2]Lawrence Livermore National Laboratory (L-280), P.O. Box 808, Livermore, California 94550, USA

Atomic forces are fundamental for using modern ab initio techniques in materials science. In this talk we propose a new methodological approach that allows to obtain atomic forces at finite magnetic temperatures solely from ab initio calculations. To demonstrate the power of the new approach we address a long standing but hitherto not solvable problem of computing phonon spectra for paramagnetic materials. As benchmark system we consider the experimentally well studied bcc and fcc phase of iron. The proposed scheme is general and an extension to study, e.g., systems containing defects (point or extended) or to combine it with molecular dynamic simulations is straightforward.