MM 8: Topical session: Integrated computational materials engineering for design of new materials II

Time: Monday 11:45–13:15 Location: H38

Topical Talk MM 8.1 Mon 11:45 H38

Modern materials design from first-principles: Recent progress and future prospects — •Blazej Grabowski — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The ever increasing demand on the performance of modern materials requires optimized design strategies. Experimental techniques alone often reach their limits and need to be supported by atomistic simulations rooted in first-principles. The great challenge is to bridge the gap between quantities accessible by simulation and quantities relevant to experiment. In this talk, I will discuss our recent progress in tackling this challenge and the implications of our work on future research, by focusing in particular on the impact of finite temperatures and microstructural complexity.

MM 8.2 Mon 12:15 H38

Characterization of deformation with various dimensionalities in $MoSi_2$ — •Mojmír Šob[1,2,3] and Martin Friák[2,1] — [1]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [2]Institute of Physics of Materials, Acad. Sci. Czech Rep., Brno, Czech Republic — [3]Department of Chemistry, Faculty of Sciences, Masaryk University, Brno, Czech Republic

We explore, with the help of ab initio electronic structure calculations, the response of molybdenum disilicide ($MoSi_2$) to a series of extreme applied loading conditions with different dimensionality. Our study is focused on energetics and structural behavior of $MoSi_2$ with tetragonal $C11_b$ structure under uniaxial, biaxial (epitaxial) and triaxial (hydrostatic) strains and stresses. Total energies and fully relaxed structural parameters are calculated by the Vienna Ab initio Simulation Package (VASP) using generalized gradient approximation (GGA). Three constrained minimum-energy paths corresponding to the uniaxial tensile test simulation along the [001] direction, biaxial stresses within the (001) plane, and triaxial loading conditions are discussed. A relaxation of both external and internal degrees of freedom is performed and their response to the different loading modes is analyzed. Studying the energy vs. strain curves, features common to all three types of strains are analyzed in accordance with the universal binding energy concept.

MM 8.3 Mon 12:30 H38

DFT-simulations of W-Be-alloys for ITER — •Jens Bröder[1,2], Martin Köppen[2], Daniel Wortmann[1], Stefan Blügel[1], and Christian Linsmeier[2] — [1]Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Energie- und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

One of the key challenges in the construction of the fusion reactor ITER lies in understanding the evolution of wall materials mostly consisting of W and Be. Here, experiments performing a chemical analysis by interpreting photoelectron spectroscopy spectra are very important. Density functional theory simulations with an all-electron code can assist by relating the measured core-level shift to the chemical environment and therefore support the evaluation of such core-level spectra. Furthermore, the simulated density of states allows the determination of the electronic properties as validated experimentally by valence-band spectroscopy.

In this talk we present calculations of core-level shifts using the FLEUR-code [1]. We use the initial-state approximation and show results for tungsten-beryllium alloys and compare them to experimental findings. In detail, we discuss the surface core-level shifts of relaxed tungsten surfaces and the chemical shifts of stable W-Be alloys.

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[1] http://www.flapw.de

MM 8.4 Mon 12:45 H38

Sampling free energies of different phases in Fe including atomic and magnetic degrees of freedom — •Martin Staadt[1], Jutta Rogal[1], Tilmann Hickel[2], Jörg Neugebauer[2], and Ralf Drautz[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The phase transition between ferrite and austenite in iron is omnipresent during manufacturing and processing of steels. Due to the combination of a structural and a magnetic transition from paramagnetic FCC to ferromagnetic BCC iron, these phase transitions are particularly challenging to investigate on the atomistic level. Previous studies were limited to embedded atom potentials that did not explicitly account for magnetism or density functional theory that proved to be too computationally expensive for a direct simulation. We overcome these limitations by using bond-order potentials that enable us to treat larger system sizes but still properly treat magnetism. Using the BOPfox code, we calculate free energies of the bulk phases and the phase boundaries with thermodynamic integration including all important contributions.

MM 8.5 Mon 13:00 H38

Thermal properties of paramagnetic α-Mn from first principles — •Hossein Ehteshami and Pavel A. Korzhavyi — Materials Technology, Deptartment of Materials Science and Engineering, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Mn is a common alloying element in steel. Therefore, its physical properties and their variation with temperature are of interest for thermodynamic modeling. α-Mn is a complex cubic phase that is stable between 0 and 1000 K and undergoes antiferromagnetic ordering below the Neel point of about 100 K. For an element with such complex crystal and magnetic structures, one can expect that the magnetic, electronic and vibrational degrees of freedom are coupled. Here we describe the paramagnetic phase of α-Mn at finite temperatures by decoupling adiabatically the "fast" (electronic and magnetic) and "slow" (vibrational) degrees of freedom. The electronic structure is calculated within the exact muffin-tin orbital (EMTO) formalism. Electronic excitations are included via finite-temperature smearing of the Fermi function. Paramagnetic disorder is treated self-consistently in the disordered local moment (DLM) model and coherent potential approximation (CPA). The so obtained partial free energies (including the electronic and magnetic contributions as functions of temperature and volume) are used as the input to the Debye-Gruneisen model of the lattice vibrations. Thermal expansion, isothermal/adiabatic bulk modulus and specific heat capacities are calculated and compared with the experimental results to demonstrate the validity of the adiabatic treatment.