MM 39: Computational Materials Modelling - Alloys I

Time: Wednesday 15:45–17:00 Location: BAR 205

MM 39.1 Wed 15:45 BAR 205

Atomistic spin dynamics coupled with *ab initio* molecular dynamics simulations of Fe in the paramagnetic state — •Davide Gambino and Björn Alling — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden

Accurate investigation of magnetic materials at finite temperatures with first principles methods is a formidable task that requires inclusion of magnetic and vibrational effects on a similar footing in order to account for their interplay. An approach that allows to investigate the coupling of these different degrees of freedom is the atomistic spin dynamics - *ab initio* molecular dynamics (ASD-AIMD) method [Stockem *et al.*, *Physical Review Letters* 121, 125902 (2018)], in which an AIMD and an ASD simulations are run in parallel communicating to each other atomic positions (which affect exchange interactions) and magnetic moments directions.

While the method was initially tested on CrN, a semiconducting system with well localized magnetic moments, in this work we perform an ASD-AIMD investigation of Fe in the paramagnetic state, close to its Curie temperature. Since Fe is a ferromagnetic metal, it is relevant to investigate also the contribution of longitudinal spin fluctuations (LSF) to the thermodynamics of the system. LSF are here included through a mean-field term derived from a semiclassical model. The present results pave the way for free-energy calculations in magnetic materials by means of *ab initio* methods.

MM 39.2 Wed 16:00 BAR 205

Disorder driven stability in Co-based Heusler compounds — •Vitaliy Romaka, Ahmad Omar, Sabine Wurmehl, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

Co-based Heusler compounds are known as promising half-metallic magnetic materials. However, their magnetic properties are affected by various factors, such as anti-site disorder, vacancies, and thermodynamic instability. Particularly in the case of systems that, in addition to Co, contain other 3*d* metals, for example Fe and/or Cr, the structural and thermodynamic issues are not very well understood. In order to shed light on the effects of structural disorder and off-stoichiometry in Co-based Heusler compounds, a section of the thermodynamic phase diagram for the quaternary Co-Cr-Fe-Al system was investigated by means of *ab initio* calculations. In the case of $Co_2Cr_{1-x}Fe_xAl$ solid solution, with energetically favorable $B2$-type structure, the shape of thermodynamic potential is quite similar to what is expected in the case of spinodal decomposition of the solid solution and is further characterized by two local minima at $x \sim 0.3$ and 0.7, which describe the binodal region. Thermodynamic instability is also observed in the $CoCr_{1-x}Al_x$ and $CoFe_{1-x}Al_x$ solid solutions. Despite the fact that the quaternary composition $Co_2Cr_{0.5}Fe_{0.5}Al$ is electronically equivalent to the thermodynamically stable Co_2MnAl phase, DFT modeling shows that the composition with higher Al content ($\sim Co_2Cr_{0.3}Fe_{0.5}Al_{1.2}$) is energetically more stable, especially at high temperatures which is consistent with the experimental data.

MM 39.3 Wed 16:15 BAR 205

Investigating anharmonicity in BCCs: from unaries to HEAs — •Prashanth Srinivasan[1], Blazej Grabowski[2], Alexander Shapeev[3], Jörg Neugebauer[4], and Fritz Körmann[1,4] — [1]TU Delft — [2]University of Stuttgart — [3]Skolkovo Institute of Science and Technology — [4]MPIE Dusseldorf

Anharmonicity is a major contributor to the vibrational free energy of metals, especially at high temperatures. It has been shown for an extensive set of FCC unaries that the anharmonic Gibbs energy contribution is positive and increases with temperature [Glensk et al., 2015]. Unlike in FCC metals, empirical works [Wallace, 2002] suggest some BCC metals to have negative anharmonic contributions to the total free energy. Computational first-principles studies beyond quasiharmonicity are, however, scarce owing to the expensiveness of such calculations. Recent advances combining efficient thermodynamic sampling schemes and machine-learnt moment tensor potential [Grabowski et al., 2019] allow for an efficient yet numerically accurate vibrational free energies determination including anharmonicity. Using this, anharmonic free energies for a set of BCC metals from unaries up to five-component multicomponent alloys are calculated and discussed. As for the unaries, the anharmonicities of different sets of alloys can show both positive as well as negative anharmonic contributions depending on alloy composition.

MM 39.4 Wed 16:30 BAR 205

Ab initio study of carbon and nitrogen interstitials in CoCrNi high entropy alloy — •Martin Zelený[1], Igor Moravčík[1], Martin Friák[2], and Ivo Dlouhý[1,2] — [1]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

Twinning-induced plasticity of CoCrNi medium entropy alloy (MEA) is responsible for its extraordinary strength-ductility-toughness combination. In present work we used density functional theory to investigate the effect of interstitial nitrogen and carbon atoms on phase stability, stacking-fault energy and magnetic properties. To describe alloys with chemical disorder as MEAs we employed directionally-optimized supercell-based quasirandom structures. We found that both elements stabilize fcc structure with respect to hcp structure which results in lower probability to create a stacking fault. On the other hand, the effect on magnetic properties is negligible.

MM 39.5 Wed 16:45 BAR 205

Magnetic ordering in Mo-based HEA — •Jakub Šebesta[1,2], Karel Carva[2], and Dominik Legut[1] — [1]Nanotechnology Centre & IT4Innovation, VŠB-TU Ostrava, 17.listopadu 2172/15 708 00 Ostrava-Poruba, Czech Republic — [2]Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5 121 16 Praha 2, Czech Republic

The multiprincipal element alloys stand for promising materials with the wide range of possible application *e.g.* in the mechanical engineering. Ones of the most known representatives are the high entropy alloys (HEA). They benefit from composing of several components, originally five (but also less), which leads to the high temperature stabilization, higher creep and oxidation resistance, improved ductility and mechanical strengths. In composition of many of them a 3d magnetic element like Cr, Mn, Fe, Co, and Ni appears. Naturally the question arises, what is the influence of such element on magnetic ordering, on the alloy stability, magnetic order and how it alter all above mentioned properties. Therefore, in this study we discuss the enhancement of the magnetic order given by a Mo substitution in the well known Cantor alloy based on ab-initio calculations employing the TB-LMTO-ASA method. This allows us to treat a disorder efficiently within the framework of the CPA. The influence of the crystal structure and the position of the Mo-substitution on the stability and the magnetic behavior is shown. The evaluation of the strength of the magnetic exchange interactions lead to the determination of T_C.