MM 13: Phase Transformations I

Time: Monday 15:45–16:45 Location: C 230

MM 13.1 Mon 15:45 C 230

Impact of magneto-chemical coupling on phase stability, vacancy formation and atomic diffusion in Fe-Cr alloys — •Hilal Bozkurt[1], Chu-Chun Fu[1], and Cyrille Barreteau[2] — [1]CEA, SRMP, Gif-sur-Yvette, France — [2]CEA, CNRS, SPEC, Gif-sur-Yvette, France

High chromium ferritic steels present a large variety of technological applications. For instance, they are promising candidate as structural materials for future fusion reactors, thanks to their strong resistance to corrosion and to radiation damage. On the other side, it is known from numerous studies that thermodynamic and kinetic properties of Fe-Cr alloys are highly sensitive to magnetism.

Despite the large amount of previous theoretical and experimental efforts, the impact of magnetism on vacancy formation and vacancy-mediated diffusion in Fe-Cr as a function of temperature and alloy composition is still unclear.

In this work, we first investigate the dependency of vacancy formation energy and migration barriers on the magnetic and chemical configuration of Fe-Cr alloys, via first principles calculations. The obtained data are then used to parameterize a spin-atomic Monte Carlo model, in order to perform simulations for an accurate prediction of equilibrium vacancy concentration and vacancy-mediated atomic-diffusion coefficients versus temperature. The specificity of the present model consists in an explicit treatment of both chemical and magnetic variables, which enables to elucidate the impact of the magneto-chemical interplay on the studied properties.

MM 13.2 Mon 16:00 C 230

Ab initio study of structure-property relations in Pb-supersaturated Sn-rich Pb-Sn alloys — •Martin Friák[1], Petr Čípek[2,1], Jana Pavlů[2], Ondřej Zobač[1], Pavla Roupcová[1,3], Ivana Miháliková[1], David Holec[4], Šárka Msallamová[5], and Alena Michalcová[5] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Rep. — [2]Masaryk University, Brno, Czech Rep. — [3]CEITEC Brno University of Technology, Brno, Czech Rep. — [4]Montanuniversität Leoben, Leoben, Austria — [5]University of Chemistry and Technology in Prague, Prague, Czech Rep.

We have performed a theoretical study of three different allotropes of Pb-supersaturated Sn-rich Pb-Sn alloys with the α-Sn, β-Sn and a simple hexagonal γ-Sn structure employing quantum-mechanical calculations. Structure-property relations were analyzed in the case of the lattice parameters, thermodynamic stability, elastic properties and mechanical stability as well as electronic-structure density of states. Compositional trends in structural, thermodynamic and electronic-structure properties were found nearly linear. Our theoretical study sheds new light on a decades-long controversy related to the γ-phase of supersaturated Sn-rich Pb-Sn alloys reported in earlier papers. We suggest that the experimental difficulties in synthesizing the γ-phase solid solutions are due to the high formation energy of this phase. A financial support received under the Project No. 22-05801S from the Czech Science Foundation is gratefully acknowledged.

MM 13.3 Mon 16:15 C 230

The impact of spin-polarization, atomic ordering and charge transfer on the stability of CoCrNi alloy — •Pavel Papež[1,2], Martin Zelený[1], Martin Friák[2], and Ivo Dlouhý[1,2] — [1]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physics of Materials, Czech Academy of Sciences, Žižkova 22, Brno, 616 00, Czech Republic

Our theoretical study analyzes the impact of atomic ordering, magnetization and ongoing charge transfer on the phase stability of the medium entropy CoCrNi alloy. The study was performed using ab-initio calculations employing simulation supercells containing 216 atoms. The supercells contained either fcc or hcp lattice sites as obtained by changing the stacking of atomic planes. For each lattice type we used six different distributions of atoms with different levels of ordering. For charge transfer analysis we employed the method developed by R. Bader. To evaluate the phase stability we have calculated the mixing enthalpy of the structures revealing differences caused by ordering. Regarding the impact of the 1st nearest neighbours (NN) on the local magnetic moments of atoms, we found clear trends in Co, Cr and Ni atoms depending on the 1st NN Cr atoms. The charge transfer exhibits similarly clear trends in which Cr releases its electrons to the two other elements and even this effect has clear dependence on Cr in 1st NN (for details see P.Papež et al., Mater. Chem. Phys. 304 (2023) 127783, https://doi.org/10.1016/j.matchemphys.2023.127783)

MM 13.4 Mon 16:30 C 230

Phase diagram of the incommensurate magnetic Hubbard model — •Liam Rampon[1], Fedor Šimkovic IV[3], and Michel Ferrero[1,2] — [1]CPHT, CNRS, École Polytechnique, Institut Polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France — [2]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France — [3]IQM, Nymphenburgerstr. 86, 80636 Munich, Germany

We present the magnetic phase diagram of the cubic Hubbard model at strong coupling. We investigate the onset of spin-spiral orderings as a function of temperature and for dopings up to 20%. By computing relevant thermodynamical potentials, we identify the leading ordering vector and discuss the mechanism that gives rise to the ordered state. We observe manifestations of the Pomeranchuk effect and also show strong evidence for a phase separation at lower temperature and doping, possibly caused by an underlying "stripe" phase. These findings were obtained with single-site dynamical mean-field theory, using a broken-symmetry formalism that allows one to directly stabilize incommesurate spiral orders.