MM 15: Computational Materials Modelling III - Bulk thermodynamics/ Phase Transitions I

Time: Monday 15:45–17:45 Location: IFW D

MM 15.1 Mon 15:45 IFW D

Impact of weak and strong magnetic coupling on the thermodynamics of chromium — •Fritz Körmann, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

Chromium is a decisive ingredient for stainless steels and a reliable understanding of its thermodynamic properties is thus indispensable. Parameter-free first-principles methods have nowadays evolved to a state allowing such thermodynamic predictions. For materials such as Cr, however, the inclusion of magnetic entropy and higher order contributions such as anharmonic entropy is still a formidable task. Employing state-of-the-art ab initio molecular dynamics simulations and statistical concepts, we compute a set of thermodynamic properties based on quasiharmonic, anharmonic, electronic and magnetic free energy contributions from first principles [1]. The magnetic contribution is modeled by an effective nearest-neighbor Heisenberg model, which itself is solved numerically exactly by means of a quantum Monte Carlo method. We investigate two different scenarios: a weak magnetic coupling scenario for Cr, as usually presumed in empirical thermodynamic models, turns out to be in clear disagreement with experimental observations. We show that only a mixed Hamiltonian including weak and strong magnetic coupling provides a consistent picture with good agreement to experimental thermodynamic data.

[1] F Körmann, B Grabowski, P Söderlind, M Palumbo, S G Fries, T Hickel and J Neugebauer, J. Phys.: Condens. Matter 25, 425401 (2013).

MM 15.2 Mon 16:00 IFW D

Thermomechanical properties of α-iron from first-principles — •Daniele Dragoni[1], Davide Ceresoli[2], and Nicola Marzari[1] — [1]THEOS - École Polytechnique Fédérale, Lausanne, Switzerland — [2]ISTM - Consiglio Nazionale delle Ricerche, Milano, Italy

Compliance tensors provide a full characterization of the mechanical response of crystals in the linear regime of stress-strain. Their prediction from first-principles is of great practical utility, given the large number of elastic constants that are not known experimentally, while also providing stringent tests for validation of electronic-structure approaches in those cases where accurate experimental numbers are available. Since the intrinsic temperature dependence of the elastic constants is determined by the vibrations of the crystal (a Bose-Einstein gas of harmonic oscillators), finite-temperature results can be computed, in the quasiharmonic approximation, from the equation of state for the materials at hand and the volume- or strain-dependence of the phonon frequencies. We use ferromagnetic bcc α-iron as a case study, carefully testing pseudopotential calculations against reference all-electron results at 0K, and cubic elastic constants at finite temperatures against experimental results.

MM 15.3 Mon 16:15 IFW D

Influence of magnetism on the stability of binary transition-metal compounds — •Alvin Noe Ladines, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Germany

Refractory elements (RE) play an important role in the development of creep-resistant ferritic steels for high temperature applications. They can act as solid solution strengthener or carbide-former but also lead to the precipitation of topologically close-packed (TCP) phases that may initiate embrittlement and fracture. It is thus important to predict the formation of TCP phases in multi-component alloys. An attempt to address this is the development of structure maps which relate the alloy stability to atomic-size difference and average band-filling of the constituents. In this study we quantify the influence of magnetism for a recently developed structure map for TCP phases of transition-metal compounds. Based on density functional theory (DFT) calculations of the heat-of-formation of TCP phases in several Fe-RE systems over the whole range of chemical composition, we derive a model that correlates the magnetic energy to the average band filling of the compounds. This can be understood within the Stoner model of itinerant magnetism where the magnetic moment on the atom corresponds to a rigid shift in the spin-polarized density of states. We rescale the structure map with respect to this shift.

MM 15.4 Mon 16:30 IFW D

Thermally stable h.c.p.-based phases in Ni-W thin films — •Sascha B. Maisel[1], Silke J. B. Kurz[2], Andreas Leineweber[2], Stefan Müller[1], and Eric J. Mittemeijer[2,3] — [1]Institute of Advanced Ceramics, TUHH, 21073 Hamburg, Germany — [2]Max Planck Institute for Intelligent Systems (formerly Max Planck Institute for Metals Research), 70569 Stuttgart, Germany — [3]Institute for Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

In this combined experimental and DFT-based study, we demonstrate that even though the Ni-W phase diagram shows no h.c.p.-based phases, h.c.p.-like stacking sequences can be observed in magnetron-cosputtered Ni-W thin films at W contents of 20 at.% to 25 at.%. The occurence of these h.c.p. domains is rationalized from first-principles calculations, showing that the vicinity of the system's ground-state line is indeed populated with metastable h.c.p.-based structures in the intermediate concentration range from 20 to 50 at.%. The h.c.p.-like stacking in Ni-W is found to be thermally stable by performing extensive XRD analysis on samples before and after heat treatments up to 850 K.

15 min break

MM 15.5 Mon 17:00 IFW D

Ab initio based insights into structural transformations and the role of interfaces in Fe-C alloys — •Xie Zhang[1,2], Tilmann Hickel[1], Jörg Neugebauer[1], Jutta Rogal[2], and Ralf Drautz[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität-Bochum, 44780 Bochum, Germany

Structural transformations in Fe-C alloys are decisive for the mechanical properties of various steels. We have combined first principles and the Solid State Nudged Elastic Band method to study the structural transformations in the Fe-C system and the role of interfaces in these processes. Our investigations revealed the occurrence of an intermediate structure, which can perfectly bridge austenite, ferrite and cementite. The formation of such a structure was found to be the result of an interfacial adaptive behavior to accommodate the misfit of lattice constants and the different magnetic states in both phases. These insights provide a detailed understanding on the origin of the complex structure of cementite and the formation mechanisms of complex microstructures such as pearlite and bainite in steels.

MM 15.6 Mon 17:15 IFW D

Atomistic simulation of transformations at disordered FeCr bcc-σ interfaces — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

We study the transformation of the σ phase in FeCr to the bcc structure. We observe disordered interface region that have a thickness of several atomic layers. Transformation paths from one crystal phase to another get obfuscated by seemingly random movements and rearrangements in the interface and create a challenge to study the transformation processes, as well as increase the computational effort of the simulation. Using coordination polyhedra and topological fingerprints we look for correlations in processes in the interface region of FeCr bcc-σ interfaces and along transformation paths trying to identify the characteristic processes responsible for the phase transition.

MM 15.7 Mon 17:30 IFW D

First-principles approach to investigate hydrogen cluster formation in austenitic Mn-rich steels — •Aurab Chakrabarty, Robert Spatschek, Tilmann Hickel, and Joerg Neugebauer — Max-Planck Institute for Iron Research, Dusseldorf, Germany

Hydrogen related failure is a well-known problem in high-strength austenitic steels for automotive applications. Experiments provide evidences of reduced ductility and H-induced local plasticity (HELP) upon H charging in these materials. The HELP model provides an explanation for the formation and propagation of cracks in austenitic steel. An important criterion for HELP is segregation of hydrogen to topological defects such as stacking faults and grain boundaries and the mechanism of H-segregation in high-Mn steels is not completely understood yet. We used density functional theory (DFT) total energy calculation to estimate the interactions between H-interstitial atoms

in Fe-Mn alloys and the influence of H on stacking faults. We observed enhanced H-H interaction in a hydrogen cluster, i.e. a local hydride phase. Furthermore, a lower solution energy provided by the presence of a stacking fault makes it a favourable site for H-accumulation. The interaction energies and elastic constants calculated using DFT are used in finite-temperature Monte-Carlo and continuum-scale analysis in order to predict a phase-diagram for a temperature driven phase separation of Fe into a dilute and a local hydride phase.