MM 26: Computational Materials Modelling IV - Phase transitions II

Time: Tuesday 11:45–13:00 Location: IFW D

MM 26.1 Tue 11:45 IFW D

Study of the austenite-martensite phase transition in steel using molecular dynamics — •Emilia Sak-Saracino and Herbert M. Urbassek — Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern

Using molecular-dynamics simulation, we study the austenite-martensite phase transition in various iron alloys. In these, we consider a dilute mixture of the alloying element (C, Ni or Cu) up to 1 at-%. The specimens are subjected to a heating/cooling cycle. The phase transition can be observed by monitoring the hysteresis of the system volume with temperature. For the alloying elements studied, we find that martensite and austenite temperatures decrease with increasing concentration, in agreement with experiment.

MM 26.2 Tue 12:00 IFW D

Atomistic simulations of solid-solid phase transformations in molybdenum — •Ari Harjunmaa[1], Jutta Rogal[1], Ralf Drautz[1], Rye Terrell[2], Sam Chill[2], and Graeme Henkelman[2] — [1]ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Department of Chemistry and the Institute for Computational and Engineering Sciences, University of Texas at Austin, Austin, Texas 78712, USA

As a refractory metal, molybdenum plays an important role in strengthening special-purpose materials such as Ni-base superalloys. In heavy usage, these materials are frequently plagued by the formation of topologically close-packed (TCP) phases, which concentrate the alloying atoms into brittle precipitates, rendering the material weaker. To find a way to prevent this detrimental occurrence, it is important to understand the atomistic processes at work in solid-solid phase transformations leading to the formation of TCP phases. As a first step, we investigate interfaces between the TCP A15 and the cubic BCC phases in molybdenum, using classical molecular dynamics to model the time evolution of the systems in question. We then compare and expand these results with those obtained from adaptive kinetic Monte Carlo simulations, extending the same system setup to room temperature; furthermore, we use this latter method to characterize singular processes involved in the transformation of the atomic layers. Finally, we evaluate the reliability of the employed empirical potential by further analysis of the main results using density functional theory.

MM 26.3 Tue 12:15 IFW D

Importance of anharmonic free energy contributions in an *ab initio* description of the hcp to bcc transition in Ti — •Dominique Korbmacher, Albert Glensk, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Ti and its alloys are a very important class of materials with various technical and medical applications. Further optimizing the properties of these alloys requires accurate and reliable phase diagrams. A recent and very promising approach is the construction of phase diagrams based on finite temperature *ab initio* simulations [1]. However, a critical and so far unresolved difficulty when dealing with Ti based systems is the dynamical instability of the Ti bcc phase at T=0 K.

In the present study, we investigate the hcp to bcc phase transition in Ti including the anharmonic contribution on a fully *ab initio* basis (density-functional theory). To overcome the long CPU simulation times typically involved in calculating anharmonicity, we use here the recently developed UP-TILD method [1]. We show that the low temperature hcp phase is well described when comparing with experimental data (e.g., heat capacity). For the high temperature bcc phase the dynamical stabilization due to phonon-phonon interaction is correctly predicted, but we show that the commonly used exchange-correlation functional (GGA-PBE) yields a too soft expansion and a too low phase transition temperature. We discuss whether alternative xc-functionals can improve the situation.

[1] B. Grabowski, et al., PRB **79**, 134106 (2009).

MM 26.4 Tue 12:30 IFW D

Simulating Order Parameters for Phase Transitions in Alloys — •Conrad W. Rosenbrock, Gus L. W. Hart, Branton J. Campbell, and Richard R. Vanfleet — Brigham Young University, Provo, UT, 84602, USA

When determining the structure of alloys using diffraction patterns, possible distortions that lower the symmetry of the parent phase can be limited by group-theoretical arguments as long as a group-subgroup relationship exists between the parent and distorted phases[1]. Order parameters are vectors in representation space where each dimension corresponds to a specific superlattice vector in reciprocal space (e.g. L = [0.5,0.5,0.5] or X=[1,0,0]); such order parameters determine the distortions that may arise during a phase transition. By measuring the Fourier transform of the structure at each relevant superlattice vector during a Monte Carlo simulation for $CuPt_3$, we were able to extract these thermodynamic order parameters and qualitatively confirm distortions in the L and X order parameters observed in experiment[2]. The methodology presents a highly effective avenue for comparing simulated phase transitions with experimental results.

[1] Harold T. Stokes, Branton J. Campbell and Dorian M. Hatch. *Order parameters for phase transitions to structures with one-dimensional incommensurate modulations*
[2] Rokuro Miida and Denjiro Watanabe. *Electron Microscope and Diffraction Study on the Ordered Structures of Platinum-Rich Copper-Platinum Alloys*

MM 26.5 Tue 12:45 IFW D

Phase-field simulation of the peritectic reaction in Al-Cu-Ni alloys — •Julia Kundin, Heike Emmerich, and Evgeny Pogorelov — University Bayreuth

The simulations of the solidification of ternary Al-Cu-Ni alloys were carried out by means of a general multi- phase-field model for an arbitrary number of phases. A realistic microstructure can be generated by coupling the real thermodynamic parameters of the phases and the evolution equations. The stability requirements for the model functions on every dual interface guarantee the absence of "ghost" phases on them. The thermal noise terms disturb the stability and can produce the heterogeneous nucleation of product phases in accordance to the energetic conditions. It is shown that the model can produce the growth of the combined eutectic-like and peritectic-like structure in various alloys. Of particular interest is the heterogeneous nucleation of the fourth phase in triple points.