MM 19: Topical Session Designing Innovative Structural Materials and Steels V

Time: Tuesday 10:15–11:15 Location: H4

Topical Talk MM 19.1 Tue 10:15 H4

Influence of pressure on decomposition thermodynamics of structural materials — •Igor A. Abrikosov[1], Björn Alling[1], Alena V. Ponomareva[2], Olga Yu. Vekilova[1], and Sergei I. Simak[1] — [1]Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden — [2]Department of Theoretical Physics, Moscow State Institute of Steel and Alloys, Moscow 119049, Russia

We show, by means of state-of-the-art theoretical simulations, that a pressure which is often present in practical applications of structural materials may have profound effect on their decomposition thermodynamics. In TiAlN, which is widely used as hard protective coating in cutting tool applications, the hydrostatic pressure enhances the tendency for isostructural decomposition, including spinodal decomposition. In Fe-Cr steels we observe a concentration reversal of pressure induced tendency towards isostructural decomposition.

Topical Talk MM 19.2 Tue 10:45 H4

Computational Phase Studies: Deriving thermodynamic properties of metals from first principles — •Tilmann Hickel — MPI für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf

In the past few years the combination of accurate first principles calculations with mesoscopic/macroscopic thermodynamic concepts has so quickly advanced, that they now allow tackling even complex engineering systems such as steels, shape-memory alloys or light-weight metals. The key for a reliable predicting also phase transitions is the availability of efficient and highly accurate theoretical tools to determine free energies from ab initio. We have therefore performed an extensive and systematic study of the capabilities of present day implementations (xc-functionals) of densitiy functional theory in determining ab initio free energies for metals. Lattice vibrations, which yield the dominant contribution to the free energy of elementary, non-magnetic materials, can be determined within the quasiharmonic approximation. We were able to show for a large set of metals that the thus derived thermodynamic properties are in excellent agreement with available experimental data. For magnetic materials such as iron we have developed a proper quantum-mechanical treatment of magnetic excitation, improving previous classical approaches. An integrated approach, combining electronic, vibrational, and magnetic effects, lead us to an extremely high accuracy of only a few meV for the free energy of the considered metals. The thus determined free energies have been successfully used to predict martensitic phase transition temperatures in selected materials such as shape memory alloys.