MM 12: Topical Session Designing Innovative Structural Materials and Steels III

Time: Monday 14:45–15:45 Location: H4

MM 12.1 Mon 14:45 H4

First principles study of thermodynamic, structural and elastic properties of eutectic Ti-Fe alloys — •Li-Fang Zhu, Alexey Dick, Tilmann Hickel, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237, Düsseldorf, Germany

Ti-based alloys have been suggested for commercial applications with a great potential due to their high strength and good corrosion resistance. The strength of these materials can be even further increased if bulk nano-structured eutectic alloys are produced. Motivated by experimental results showing eutectic Fe-Ti alloys decomposing into the FeTi compound with B2 structure and β-Ti alloys with varying Ti concentration, Ti-Fe alloys covering a broad range of Ti concentrations were studied using density functional theory within generalized gradient approximation. Our formation energies correctly predict the experimentally observed phases and we explain their stability in terms of a sensitive concentration dependence of the density of states at the Fermi level. Further, single-crystalline elastic constants as well as polycrystalline moduli are predicted employing Hershey's homogenization. Based on these results we discuss the effect of local lattice strain on the thermodynamic phase stability and elastic properties in nano-structured eutectics.

MM 12.2 Mon 15:00 H4

Importance of magnetic effects on structural properties in Al- and Si- substituted Laves phases Fe_2Nb and Fe_2W — •François Liot, Martin Friák, and Jörg Neugebauer — Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Laves phases are promising candidates for the design of new steels with superior mechanical strength. Here we study systematically thermodynamic, structural and magnetic properties in Al- and Si- substituted Laves phase compounds Fe_2Nb and Fe_2W using first-principles density functional methods. Spin polarized calculations predict that substituting Al atoms for Fe atoms in Fe_2Nb is energetically more favorable than substituting Al atoms for Nb atoms. Furthermore, they show that this leads to a significant increase of the lattice constant along the a axis. To investigate the effects of magnetism, non-magnetic calculations are carried out for the same Fe-Nb-Al compounds. Our results show that the inclusion of magnetism is crucial to accurately reproduce experimental data. Based on this insight, theoretical predictions for ternary alloys Fe-Nb-Si, Fe-W-Al and Fe-W-Si are presented.

MM 12.3 Mon 15:15 H4

The influence of interstitial carbon and substitutional Nb-Mo on the mechanical properties of Ti-Al - an ab initio study — •Dominik Legut[1,2], Juergen Spitaler[1,2], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Leoben, Austria — [2]Materials Center Leoben, Leoben, Austria

Ti-Al based alloys exhibit very attractive properties such as low density, high strength at high temperatures, and very good oxidation resistance, but they are brittle at room temperature. Addition of transition elements or elements like carbon, nitrogen and oxygen can significantly improve their behavior regarding strength and ductility. We perform first-principles calculations based on density functional theory to investigate the influence of interstitial carbon on the energetics of both, the α_2 ($L1_0$) and γ (DO_{19}) structure of this alloy. The elastic constants of Ti-Al alloys with interstitial carbon are calculated and compared to the results for the pure α_2 and γ Ti-Al phases. Moreover, we study the quaternary system Ti-Al-Nb-Mo, where we determine the positions of Nb and Mo with respect to each other. Also the heat of formation is predicted for Nb-Mo concentrations which resemble the real alloy compositions.

MM 12.4 Mon 15:30 H4

Atomistic studies of dislocations in α-iron using bond-order potential — •Matous Mrovec[1,2], Christian Elsässer[1,2], and Peter Gumbsch[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]IZBS, Universität Karlsruhe, Karlsruhe, Germany

Macroscopic plastic behavior is closely linked to properties of dislocations at the nanometer scale. Direct experimental observations of the dislocation core region and of its changes during dislocation motion are unfortunately impossible and better understanding of these phenomena can be obtained only with the help of atomistic simulations. Recent atomistic studies of dislocations in iron have provided however very different outcomes, both in terms of atomic structures and energetics. The most likely reason of these large differences is a lack of reliable interatomic potentials, which would be able to describe adequately the atomic bonding and magnetic interactions in iron.

In the present work we present studies of dislocations in α-iron using a bond-order potential, which is based on a tight-binding bond representation. The model is able to capture the directional character of bonds present in transition metals and includes a description of magnetic effects within the Stoner model of itinerant magnetism. We will compare results of our simulations with available first-principles predictions as well as with predictions of other empirical interatomic potentials and discuss underlying causes of the differences.