MM 28: Topical Session Theory meets Experiment I - Intermetallics and Steels

Time: Wednesday 10:15–11:30 Location: TC 006

Topical Talk MM 28.1 Wed 10:15 TC 006

Some Contributions to Materials Design from Combined Three Dimensional Observation of Materials by Atom Probe Tomography and Three Dimensional Atomistic Modelling — •George Smith — Department of Materials, Oxford University, Parks Road, Oxford OX1 3PH, United Kingdom

Two exciting new developments have come together in recent years in the field of materials science. For the first time, we are able to observe experimentally the three-dimensional atomic-scale chemistry of solids, by atom probe tomography. Also, we are now able to carry out large-scale computer modelling of materials in three dimensions at the atomic level. The combination of experiment and theory opens totally new horizons for intelligent materials design and development. Three case studies, from very different fields, will be presented to illustrate the power of this new approach. The first relates to the development of improved pressure vessel steels for energy generation. The second involves the improvement of manufacturing methods for magnetic sensors for use in computer memories. And the third demonstrates the use of atomic-scale imaging and analysis to assist in optimising the activity of core-shell nanoparticle catalysts for fuel cell applications.

MM 28.2 Wed 10:45 TC 006

Decomposition of cementite under strain in pearlitic steels: An ab intio study — •Gholamali Nematollahi, Johann von Pezold, Jörg Neugebauer, and Dierk Raabe — Max-Planck Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Severely plastically deformed pearlitic wires are amongst the strongest materials known to mankind. Despite extensive research the fundamental mechanisms underlying the extraordinary strength of this α-Fe/Fe3C composite are still unclear. Experimental evidence suggests that the applied strain induces a substantial migration of C atoms from cementite lamellae into adjacent ferrite particles, resulting in a dramatically increased C concentration in the ferrite matrix after the plastic deformation (by ~ 9 orders of magnitude). We therefore consider here the stability of C interstitials in ferrite and of C vacancies in cementite as a function of the relevant strain state, using density functional theory. Our analysis reveals a substantial strain-induced stabilization of the C interstitial in ferrite and a minor destabilization of the C vacancy in cementite. Using this insight we are able to explain the experimentally observed partial dissolution of cementite in severely plastically deformed pearlitic wires by the strain-induced stabilization of C interstitials in ferrite.

Keywords: Density functional theory, Ferrite, Cementite, Carbon interstitial, vacancy formation energy

MM 28.3 Wed 11:00 TC 006

On the dependence of elastic properties on the point-defect content in vacancy-rich β-NiAl — •Sascha B. Maisel and Stefan Müller — Insitute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

The high-temperature alloy β-NiAl can tolerate an exceptionally high number of point defects in the form of vacancies or anti-site atoms. In fact, the B2 phase which $Ni_{50}Al_{50}$ prominently exhibits is still stable up to vacancy-rich crystals with a stochiometry of around $Ni_{42.5}Al_{50}$ [Warlimont77]. However, we find that many assumptions that are commonly used when describing the dependence of elastic constants on point defects in single crystals do not hold for β-NiAl. In particular, the Wagner-Schottky approximation is not valid and common analytical descriptions [Pistorius70] fail due to cell volume changes at high vacancy contents. Moreover, the widely used five parameter extrapolation [Warlimont77] for the elastic moduli in β-NiAl is not correct for very high defect concentrations. We present improved values for the elastic behavior in the high-vacancy regime derived from fully relaxed first-principles structures.

References:
N. Rusovic, H. Warlimont: Phys. Stat. Sol. 44, 609 (1977)
M. Pistorius: Z. angew. Phys. Z9, 145 (1970)

MM 28.4 Wed 11:15 TC 006

Understanding H-induced failure mechanisms in metallic alloys: The role of attractive H-H interactions in nano-precipitate formation — •Johann von Pezold, Alexander Udyansky, and Joerg Neugebauer — Max Planck Institut fuer Eisenforschung GmbH, Duesseldorf

Attractive H-H interactions have recently been shown to induce the formation of local hydride precipitates even in non-hydride forming matrices, such as Ni [1]. The formation of these nano-hydrides in the strain field of lattice defects such as crack tips and dislocations has been correlated to the long-standing problem of hydrogen embrittlement in these metals. In this study we systematically investigate H-H interactions in a range of fcc matrices, including Ca, Mn, Fe, Co, Ni, Al and Pd, using density functional theory. While the interaction between H atoms in first nearest neighbour interstitial sites is generally attractive, the nature of this interaction is strongly system and site dependent. Hence, the interaction between octahedral sites is predominantly of elastic nature, while interactions between tetrahedral sites exhibit a significant chemical contribution. Based on this study the formation of nano-hydrides in fcc metals will be critically discussed.

[1] J. von Pezold, L. Lymperakis and J. Neugebauer, Acta Mat. 59, 2969 (2011).