

## MM 20: Topical Session Designing Innovative Structural Materials and Steels VI

Time: Tuesday 11:30–13:00

Location: H4

MM 20.1 Tue 11:30 H4

**Ab initio analysis of the carbon solubility limits in various iron allotropes** — OLGA KIM, ●MARTIN FRIÁK, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 402 37, Düsseldorf, Germany

The solubility limits of carbon in various iron phases are of critical importance for many steel-industry applications. The actual values are difficult to measure accurately in ferrite and they have so far not been determined theoretically from first principles in austenite. The solubility limits of carbon in  $\alpha$ ,  $\beta$ ,  $\gamma$ , and  $\delta$  iron have been thus determined employing density functional theory calculations over the entire temperature range. The results show excellent agreement with experiment. The two-orders-of-magnitude higher solubility of carbon in austenite than in ferrite has been quantitatively analyzed and a complex interplay between two distinct phenomena has been found. First, the number of first nearest neighbors is higher in the fcc structure than in the bcc structure and the carbon atom is consequently more strongly bound, and secondly, the strain energy between the C-interstitial and the surrounding iron matrix is lower in the fcc lattice. The details of the actual magnetic state have not been found as important as the above mentioned two mechanisms.

MM 20.2 Tue 11:45 H4

**Multi-scale study of martensite stability in Fe-based solid solutions** — ●ALEXANDER UDYANSKY, JOHANN VON PEZOLD, ALEKSEY DICK, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany  
Martensitic phases refer to tetragonal states of interstitial solid solutions. We study such Fe-based dilute phases by combining atomistic modeling with the reciprocal space microscopic elasticity theory (MET), which allows us to account for long-ranged elastic interactions between impurities. The short-range chemical interactions, as well as the parameters entering the MET are obtained by density functional theory (DFT) calculations. This approach allowed us to compute temperature/interstitial concentration phase diagrams and provided a direct insight into the stability limits and formation mechanisms of martensite: specifically, tetragonal states are predicted to be preferred even at low impurity concentrations of carbon, nitrogen and oxygen due to a thermodynamically driven orientational ordering of the interstitials. Moreover, both the structural type of the tetragonal state and the transition temperature were found to sensitively depend on the local strain state of the system.

MM 20.3 Tue 12:00 H4

**Ordering and precipitation in Ni-rich Ni-W and Ni-Re** — ●NILS SCHINDZIELORZ, KATHARINA NOWAK, and STEFAN MÜLLER — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudstr. 7, D-91058 Erlangen

The unusual high hardening effect of Re compared to that of W when alloying them to Ni-based superalloys has already been discussed to be caused by the formation of precipitates within the Ni matrix [1]. By the combination of a density functional theory based cluster expansion Hamiltonian with Monte-Carlo simulations using the programme package UNCLE [2] it will be shown that for Ni-Re in the dilute limit with concentrations less than 10 at. % precipitates with a D1a structure emerge within the  $\gamma$  phase whereas for Ni-W the dominant effect is the formation of solid solutions. The interpretation of the calculated short range order patterns clarifies these results. However, for less than 5 at. % also in Ni-W indications can be found for the formation of precipitates.

Supported by Deutsche Forschungs-Gemeinschaft.

[1] J.Rüsing et al., Scripta Materialia **46** (2002) 235-240

[2] D.Lerch et al., Modelling Simul. Mater. Sci. Eng **17** (2009) 055003 (19pp)

MM 20.4 Tue 12:15 H4

**New structure maps for topologically close-packed phases in Ni-based superalloys** — BERNHARD SEISER<sup>1</sup>, THOMAS

HAMMERSCHMIDT<sup>2</sup>, ●RALF DRAUTZ<sup>2</sup>, and DAVID G. PETTIFOR<sup>1</sup> — <sup>1</sup>Department of Materials, University of Oxford, Oxford, United Kingdom — <sup>2</sup>ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Refractory elements like Re and W are added to Ni-based superalloys to improve the creep resistance. It is observed that too large concentrations induce the formation of topologically close-packed phases (TCPs) that destroy the single-crystal lattice of the Ni-based superalloys and are detrimental to the mechanical properties. In this talk we will present analytic bond-order potentials that are suitable for the prediction of TCP phase stability. By using the moments theorem that relates the crystal structure to the electronic density of states, the analytic interatomic bond-order potentials are obtained by expanding the tight-binding electronic structure in terms of response functions that depend on the Fermi energy and moments of the density of states that are given as functions of the local atomic environment. With the help of the analytic bond-order potentials the structural stability of TCP phases is then characterized as a function of valence-electron count and lattice structure. For example, at the fourth moment level we observe a distinct separation of the TCP phases in two groups. Based on the analysis of the stability of the TCP phases as a function of size difference and valence-electron count, we propose a new structure map that separates the TCP phases in different regions of stability. We compare the predictions of the structure map to DFT calculations.

MM 20.5 Tue 12:30 H4

**Entropic stabilisation of topologically close-packed phases in binary transition-metal alloys** — ●THOMAS HAMMERSCHMIDT<sup>1</sup>, BERNHARD SEISER<sup>2</sup>, SUZANA G. FRIES<sup>1</sup>, INGO STEINBACH<sup>1</sup>, RALF DRAUTZ<sup>1</sup>, and DAVID G. PETTIFOR<sup>2</sup> — <sup>1</sup>ICAMS, Ruhr-Universität Bochum, Bochum, Germany — <sup>2</sup>Department of Materials, University of Oxford, Oxford, United Kingdom

The formation of topologically close-packed (tcp) phases in Ni-based superalloys leads to the degradation of the mechanical properties of the alloys. The precipitation of the tcp phases is attributed to refractory elements that are added in low concentration to improve creep resistance. It is well known that the structural stability of the tcp phases A15,  $\sigma$  and  $\chi$  is driven by the average d-band filling. For a direct comparison to experimental phase diagrams, we carried out extensive density-functional theory (DFT) calculations of the tcp phases A15, C14, C15, C36,  $\mu$ ,  $\sigma$ , and  $\chi$  in tcp-forming binary transition-metal (TM) systems. We observe several systems such as W-Re with positive values of the heat of formation for all tcp phases although some of the phases are observed experimentally. By combining our DFT total energies with the CALPHAD methodology, we can demonstrate that configurational entropy can stabilise the tcp phases in these systems.

MM 20.6 Tue 12:45 H4

**Anomalous thermal expansion in iron-nickel alloys: ab initio calculations and the relation to magnetism** — ●FRANÇOIS LIOT<sup>1</sup> and CHRIS HOOLEY<sup>2</sup> — <sup>1</sup>Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — <sup>2</sup>Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, U.K.

The thermal expansion of ferromagnetic disordered iron-nickel alloys at various temperatures is studied, using an approach based on Ising magnetism and first-principles calculations of the disordered local moment (DLM) type. The theory correctly describes the strong increase of the thermal expansion coefficient with increasing nickel concentration from 0.35 to 0.8 at room temperature. It also reproduces the Invar effect for  $x = 0.35$ . These results are analyzed, and the effect of the magnetic free energy contribution on the thermal expansion is discussed. Furthermore, a simple relationship between anomalous thermal expansion and magnetism is presented. It is argued that an alloy shows the Invar effect if the concentration of nearest-neighbor iron-iron pairs with anti-parallel local moments increases sufficiently rapidly with temperature over a broad temperature interval.