MM 10 Intermetallic phases

Time: Monday 16:30–17:45 Room: IFW D

MM 10.1 Mon 16:30 IFW D

Anomalous equilibrium volume change of magnetic Fe-Al crystals — •Martin Friák and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany

Iron aluminides represent a very promising class of intermetallic materials with great potential for substituting stainless steels at elevated and high temperatures. Recent experiments observed an anomalous equilibrium-volume behaviour as a function of concentration in Fe-rich compounds [1]. This effect has been tentatively assigned to be due to an order-disorder transition.

In order to clarify this point we have studied the role of magnetism in Fe-Al crystals employing density functional theory (DFT) within the generalized gradient approximation (GGA). The excess energies, equilibrium lattice parameters and magnetic states have been determined for a dense set of different iron concentrations and a large variety of atomic configurations. Both external and internal relaxations were allowed.

The spin-polarized calculations for *ordered* ferromagnetic Fe-rich compounds nicely reproduce the anomalous volume behaviour, i.e. the effect is *not* related to an order-disorder transition. Analyzing different magnetic states we identified the change in magnetism to be the driving force. In fact, performing the same calculations but switching off magnetism removed the anomalous volume dependence and showed a clear linear dependence. Based on these results the importance of order-disorder transition in Fe-Al systems is revisited.

[1] R. A. Buckley and S. Kaviani, *Mat. Sci. Eng.* **A258**, 173 (1998).

MM 10.2 Mon 16:45 IFW D

Detecting low-temperature intermetallic compounds in the Ag-Pd-system - a first principles study — •E. Winning, S. Bärthlein, and S. Müller — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

Similar to Cu-Pd and Au-Pd, Ag-Pd-compounds form long-periodic superlattices (LPS) based on the $L1_2$-structure at 25at.% Pd. Experimentally Ag-Pd is known to form mutually miscible disordered solid solutions down to $\sim$ 800 K, but at lower temperatures no experimental data is available up to now. With the help of total-energy DFT calculations and a mixed-space cluster-expansion (MSCE) in conjunction with genetic algorithms (GA) [1], effective multi-body interactions are designed, that permit us to study millions of possible ground-states (GS) over the full concentration range. We thus find some new GS compared to earlier studies [2]. Most notably we predict the LPS3 as GS at $x_{Pd} = 0.25$. At $x_{Pd} = 0.5$ we can confirm earlier results by also predicting $L1_1$ as ground state, although a similar structure lies almost degenerately above. Like in the case of Cu-Pd 2D- and 3D-LPS are taken into consideration to confirm the LPS3-structure as GS. By applying Monte Carlo simulations we predict the phase transition temperatures and the short-range order behaviour.

[1] G.L.W. Hart et al., Nat. Mater. **4**, 391 (2005)
[2] S. Müller and A. Zunger, Phys. Rev. Lett. **87**, 165502 (2001)

MM 10.3 Mon 17:00 IFW D

Electric conductivity of long-range ordered FeAl alloys clarified by ab-initio calculations — •Wilfried Wunderlich[1], Raimund Podloucky[2], Wolfgang Püschl[3], and Wolfgang Pfeiler[3] — [1]Nagoya Institute of Technology, Japan — [2]Institut für Physikalische Chemie, Universität Wien — [3]Institut für Materialphysik, Universität Wien

Complicated resistivity behaviour in near-stoichiometric FeAl was interpreted as a transient establishment of local order on the way to a homogeneous equilibrium state of long-range order. In order to get more insight into the resistivity of short-range and long-range ordered states in this material, ab-initio studies were performed by extending previous band structure calculations from the literature. Spin-dependent VASP calculations were done for FeAl model crystals both defect-free and containing vacancies and antisite defects. From the curvature of bands near the Fermi level the effective electron mass was determined. The results are discussed in the framework of the Kubo-Greenwood formalism with reference to the experimental findings.

MM 10.4 Mon 17:15 IFW D

The Re-containing Inconel 706 Alloy: 3DAP Measurements — •Vitaliy Kindrachuk[1], Nelia Wanderka[1], John Banhart[1], Dominique Del Genovese[2], and Joachim Rösler[2] — [1]Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany — [2]Institut für Werkstoffe, TU Braunschweig, Langer Kamp 8, 38106 Braunschweig, Germany

Inconel 706 is a wrought Ni-Fe base superalloy which is used for applications at service temperatures up to 600°C. The good mechanical properties are caused by precipitation of intermetallic phases γ' (L12 structure) and γ'' (DO22 structure). Re is known to stabilize the microstructure of Ni-based superalloys at higher temperature. Therefore, the influence of Re on Inconel 706 was investigated in the present study.

The microstructure evolution of 0.6 at.% Re-alloyed Inconel 706 was studied after ageing at 750°C for 750 h and 5000 h by three-dimensional atom probe tomography and by TEM.

The modified stabilization heat treatment (MST) produces individual γ' and γ'' precipitates and γ'/γ'' co-precipitates with average sizes of about 15 nm. Re concentrates mostly in the matrix (about 0.8 at. %), whereas the intermetallic phases contain 0.2 - 0.3 at.%. Large γ'' plates with sizes of about 50 - 100 nm are formed after ageing at 750°C for 750 h. Their Re-content is very small (0.07 at.%).

After ageing for 5000 h only one type of precipitates remains, namely η plates embedded into the matrix. Therefore, the Re-alloyed Inconel 706 loses its mechanical properties. Unexpectedly Re does not stabilize the microstructure of the alloy at 750°C.

MM 10.5 Mon 17:30 IFW D

Metastable phase formation in Ti-Al-Nb undercooled melts — •Olga Shuleshova, H-Günther Lindenkreuz, Regina Hermann, Thomas George Woodcock, Wolfgang Löser, and Bernd Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Metastable phase formation processes in ternary Ti-Al-Nb turbine blade alloys have been studied by containerless electromagnetic levitation for melt undercooling up to 300 K below the liquidus temperature. The recalescence behaviour of $Ti_{45}Al_{45}Nb_{10}$ indicates β-phase formation with subsequent β to α transformation, whereas from the double-recalescence events of $Ti_{40}Al_{50}Nb_{10}$, $Ti_{45}Al_{50}Nb_5$ melts metastable β-phase formation is inferred beyond critical undercooling in the range of 150 K. Dendrite growth velocities of 10 to 20 m/s for highly undercooled Ti-Al-Nb melts are consistent with primary β-phase formation, which is promoted by Nb addition. For $Ti_{45}Al_{50}Nb_5$ and $Ti_{40}Al_{50}Nb_{10}$ alloys a second recalescence near 1300°C attributed to an α to γ solid state transformation was observed in the pyrometer trace. The γ-phase formation was suppressed in favour of a homogeneous α_2-phase in undercooled $Ti_{45}Al_{45}Nb_{10}$ samples quenched onto a chill substrate. Whereas, in $Ti_{40}Al_{50}Nb_{10}$, high undercooling enabled a direct γ-phase solidification.