MM 37: Intermetallic Phases II

Time: Thursday 10:15–11:15 Location: H 0111

MM 37.1 Thu 10:15 H 0111

In situ electrochemical nanoindentation: A nanomechanical approach to environmental degradation of iron aluminium — •Afrooz Barnoush, Christian Bies, and Horst Vehoff — Saarland University, Departement of Materials Science, Bldg. D22. P.O. Box 151150, D-66041 Saarbruecken, Germany

New nanomechanical testing methods such as nanoindentation allow us to study mechanical properties and deformation processes on the nanoscale. However, engineering materials are employed and operated under corrosive environments which are not easy to simulate inside of sensitive instruments like the nanoindenter. This was the motivation for constructing a new in-situ electrochemical nanoindentation setup, which is used to study the effect of environment on the deformation of FeAl single crystals in comparison to other metals. Especially the effect of the environment and surface films on dislocation nucleation and multiplication should be studied. For this the electrochemical setup is integrated into a nanoindentation system. By changing the electrochemical potential, a variety of different environments are able to be simulated during the indentation tests. The results show strong influence of the environment on the mechanical properties. Furthermore, the environmental effects on dislocation nucleation inside the material are investigated by analyzing the yield point phenomena (pop-in) in load-displacement curves. Recent results will be presented in the talk.

MM 37.2 Thu 10:30 H 0111

Combined experimental and ab-initio investigation of the physical properties of Ni_3Ge and Ni_3Al — Markus Dinkel, Rebecca Janisch, •Florian Pyczak, and Mathias Göken — Institute General Materials Properties, University Erlangen-Nürnberg, Erlangen, Germany

Germanium is a promising element for brazing alloys to repair single crystalline ni-base superalloys. Germanium has the advantage that it forms an ordered Ni_3Ge phase with the same crystal structure as Ni_3Al (γ' phase). The γ' phase is responsible for the excellent mechanical properties of ni-base superalloys at high temperature. Interdiffusion between the braze and the base material causes a decreasing concentration of germanium from the brazing zone to the base material and vice versa for aluminum. In the γ' precipitates germanium is more and more substituted by aluminum, which should lead to changing properties of the γ' phase between brazing zone center and base material.

In our investigations we determined the chemical composition of binary Ni-Ge by energy dispersive spectroscopy in the electron microscope, the lattice constants using X-ray diffraction investigated the mechanical properties by nanoindentation in an atomic force microscope.

Additionally, equilibrium lattice constants, energies of formation, bulk moduli and defect energies of pure Ni_3Ge and Ni_3Al phases were calculated by means of a spin-polarized ab initio density-functional method in the general-gradient approximation. The results will be discussed in the light of the experimental data.

MM 37.3 Thu 10:45 H 0111

Determination of order parameters and site occupation by means of Atom Probe Tomography — •Torben Boll[1], Talaat Alkassab[1], Zhi-Guo Liu[2], and Lei Shi[1,2] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Laboratory of Solid State Microstructures, Nanjing University, Hankou Road 22, Nanjing 210093, China

An algorithm, that uses statistical methods for the determination of site occupation and order parameters, was developed and applied on various samples.

These samples, consisting of dual phase α_2/γ-TiAl-specimen ($L1_0$-structure) with Additions of either 3at.%Cr, 2at.% Ag or 1-10at.% Nb were produced by means of leviation melting, respectivly. For comparison within this study a standard intermetallic phase of CuAu was fabricated as well.

The Atom Probe Tomography (APT)-results are presented and compared with X-Ray-Diffraction (XRD) and Atomic Location by Channeling-Enhanced Microanalysis (ALCHEMI).

Field ion Microscopy (FIM) images allow general statements about site occupation, if assumptions about the imaging behavior of the involved elements are made. Concerning the order it is only possible to state, whether the sample is well ordered or not.

In contrast, with the developed APT-algorithm it is furthermore possible to attain information about the field evaporation field strengths of the different components in the respective unit cells.

MM 37.4 Thu 11:00 H 0111

Stability range of the B2 NiAl phase investigated by a ternary Cluster-Expansion — •Daniel Lerch, Kerrin Dössel, and Stefan Müller — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

The strongly ordering B2 phase of the intermetallic compound NiAl is known to be stable for a broad concentration range off its ideal 1:1 stoichiometry. Evidently this is due to the existence of constitutional defects. Experimental studies have shown that the dominant defect types in Al rich and Al poor parts of the B2 phase are Ni vacancies and Ni antisites (Ni atoms on the Al sublattice) respectively.

We have performed an ab-initio study using a ternary cluster-expansion (*CE*) based on density functional theory (*DFT*) calculations. In connection with Monte-Carlo methods, this is an excellent tool to elucidate short-ranged order of defects at finite temperatures, which will be presented here. The results give rise to doubts, whether the stability region of B2 NiAl is indeed as broad as shown in phase diagrams.

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