MM 8 Symposium Modern Metallic Materials Design II

Time: Monday 14:45–16:30 Room: IFW B

MM 8.1 Mon 14:45 IFW B

Investigation of the phase boundary and site occupation of atoms in pure and doped TiAl/Ti3Al intermetallic by means of the tomographic atom probe (TAP) — •Torben Boll[1], Talaat Al-Kassab[1], Yong Yuan[2], and Zhi-Guo Liu[2] — [1]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Laboratory of Solid State Microstructures, Nanjing University, Hankou Road 22, Nanjing 210093, China

Dual-phase TiAl/Ti3Al alloys consisting of a lamellar structure, comprising γ-phase plus a small amount of $\alpha 2$-phase, with addition of 1 and 5at.%Nb were prepared. The samples were investigated by means of the field ion microscopy (FIM), the tomographic atom probe (TAP) and supporting TEM, HRTEM analysis. The influence of Nb-alloying on the variation of the field evaporation and microstructural parameters in the γ-phase as studied by FIM and TAP will be reported in this contribution. A new data treatment approach based on TAP results was developed to evaluate the site occupancies in such ordered structures. The Nb-atomic site occupancies, as well as any clustering and/or ordering of Nb atoms will be reported. In addition, computer modeling and simulation of the field evaporation behavior of the different species including the next neighbor interaction in a FIM specimen are performed for the first time. From these simulations, a structural order parameter and binding energies for the different species can be estimated. A comparison of the results, obtained with this model, to the experimental data will be presented and discussed for the site occupancy of Nb in these alloys.

MM 8.2 Mon 15:00 IFW B

Computer simulation of the field evaporation in TiAl with additions of Nb — •Torben Boll[1], Talaat Al-Kassab[1], Yong Yuan[2], and Zhi-Guo Liu[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

The formation of an image in the field ion microscope and subsequently the field assisted evaporation of the upper most surface atoms from the atomic layers as originated in the tomographic atom probe were simulated. As a model system we have selected the ordered structure of the γ-TiAl-phase with a $L1_0$-unit cell containing various additions of Nb. For the first time in such a computer modeling next neighbor (NN)-binding energies have been used. The effect of site occupation and concentration of Nb on the process of field evaporation and its influence on the TAP- and FIM-results were investigated as well. Further algorithms were developed to explore the vicinity around selected species and hence to analyze the degree of order based on TAP results. These processes were tested on experimental as well as on simulated data. In this contribution the computer model will be presented and discussed. In particular the focus will be emphasized on the approach to estimate NN-binding energies and order parameters by comparing the simulations with experimental data.

MM 8.3 Mon 15:15 IFW B

TEM investigations of TiAl-based intermetallic compounds — •Yong Yuan[1], Zhi-Guo Liu[1], Torben Boll[2], and Talaat Al-Kassab[2] — [1]Laboratory of Solid State Microstructures, Nanjing University, Hankou Road 22, Nanjing 210093, China — [2]Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

TiAl based intermetallic alloys are promising high-temperature structural materials. Nb addition can enhance the strength, and precipitation hardening can improve the strength and creep-resistance of the alloys.

Dissociation of super-dislocations in Ti-48at.%Al-1at.%Nb and Ti-48at.%Al-10at.%Nb has been studied by HRTEM. Corresponding superlattice intrinsic stacking fault (SISF) energies in γ-TiAl were determined to be about 63 mJ/m^2 and 34 mJ/m^2, respectively. It is concluded that Nb addition can decrease the SISF energy, which may contribute to the strengthening effect. The microstructure of Ti-48 at.% Al-10 at.% Nb aged at 1073 K was also investigated by TEM. Needle-like $\gamma 1$-$Ti_4Nb_3Al_9$ precipitates in the γ-TiAl matrix predicted before were for the first time observed. Their morphology and the orientation relationship was characterized.

The precipitation reaction of $L1_2$-$(Al,Ag)_3Ti$ in an $L1_0$ -TiAl(Ag) based Ti-54at.%Al-2at.%Ag alloy has been studied by TEM, HRTEM and supporting micro-hardness test preliminarily. The maximum hardness appeared in the samples with an average precipitate diameter of about 40 nm. The morphological evolution of the precipitates was discussed.

MM 8.4 Mon 15:30 IFW B

Monte-Carlo-Simulation of Nucleation of GP-Zones in Al-Cu-Alloys — •Andreas Lammerschop, Volker Mohles, and Günter Gottstein — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen, Kopernikusstr. 14, 52056 Aachen

Age-hardening by precipitation is one of the most important mechanisms for strengthening of Al-alloys. We present an atomistic Monte-Carlo-Model for calculations on an f.c.c.-lattice. Diffusion is implemented by a vacancy mechanism. The thermodynamic driving force is represented as a regular solution model based on the bonding energies of the nearest and next nearest neighbours. The elastic energy model is based on the concept proposed by Eshelby and Khachaturyan. As to be expected from experiments, the simulations show that precipitations nucleate parallel to {100}-planes. This is actually caused by the elastic energy. In these MC-simulations, the thermodynamic energetics used have been based on experiments. The coupling of this model with quantum theory calculations (DFT) will improve the understanding of the formation process. Moreover it will enable true predictions on the precipitation kinetics in other f.c.c.-alloys.

MM 8.5 Mon 15:45 IFW B

First-principles studies on the precipitation thermodynamics of Al-Cu alloys — •Shaoqing Wang and Hengqiang Ye — Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

The technique of precipitation hardening is widely used for strengthening alloy materials in metallurgical industry. We studied the structure and ground-state energetics of Guinier-Preston (GP) precipitates in Al-Cu alloys. An atom-scale mechanism for the formation and structure evolution of GP zones in Al-Cu alloys was proposed [1]. The precipitation is a thermodynamic phenomenon. For a thorough understanding of the matter, it is essential to investigate the thermodynamic aspect of the process. In present work, we study the precipitation thermodynamics of Al-Cu alloys by first-principles response-function calculation [2]. The optimized atomic configurations of Al-Cu superlattices [1] for different Cu content are adopted as the starting point. We firstly calculate the dynamical matrices of Al-Cu superlattices for a set of special q-points. Then the full phonon spectrum is obtained by the Fourier interpolation algorithm of dynamical matrices [3]. From these full phonon spectrums, the temperature dependences of Helmholtz free energy and entropy of these Al-Cu superlattices are calculated. The structure evolution of GP precipitation as temperature decreases is reasonably interpreted.

[1] S. Q. Wang, M. Schneider, H. Q. Ye, G. Gottstein, Scripta Mater. 51, 665 (2004).
[2] X. Gonze, Phys. Rev. B 55, 10337 (1997).
[3] S. Baroni et al., Rev. Mod. Phys. 73, 515 (2001).

MM 8.6 Mon 16:00 IFW B

Are Guinier-Preston Zones in Al-Alloys stabilized by GrowninStructural Vacancies — •Torsten E.M. Staab, Michael Roebel, and Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik,Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16,D-53115 Bonn, Germany

Aluminum alloys obtain their strength by nanometer-sized precipitations of their alloying elements, which are effectively hindering the dislocation motion. The morphology of precipitations varies from spherical via ellipsoidal to plate- or needle-like structures. Recent ab-initio calculations on a plane of 14 Cu atoms – not containing any vacancies – in aluminum showed that this structures are unstable [1]. However, structural vacancies may be found in precipitations as-grown after solution heat treatment, quenching to water, and subsequent ageing. By the SIESTA ab-initio code we calculate the formation energies for vacancies in aluminum and their binding energy to substitutional atoms of the alloying elements for Al-Ag, Al-Cu and Al-MgSi. Additionally, we determine the formation and binding energies for vacancies inside the precipitations in

these materials, since important classes of technical alloys used in outer shell plates of airplanes are based on AlCu or AlMgSi. The results of the ab-initio calculations will be compared to positron annihilation experiments on AA2024 and AA6013 alloys.
[1] M. Röbel, Dissertation University Bonn, 2005

MM 8.7 Mon 16:15 IFW B

Analyse of frequency spectrum in the austenitic steel sample — •Remus Zagan, Petre Petculescu, and Niculae Peride — Ovidius University of Constanta, Mamaia Ave. 124, 900527, Constanta, Romania

This paper presents some experimental results in order to evaluate the effect of wavelet transform (WT) filtering on ultrasonic spectral analysis. By applying WT, the authors proved that it is possible to compress and filter the ultrasonic signal buried in noise, without any loss of accuracy in the time measurement. The experiments were made on an austenitic stainless steel sample 16Mo3. For the peak frequency the following values were found: 4.11 MHz by power spectrum (PS) and 4.111 MHz by power spectrum density (PSD). In this paper, we have used the power spectrum (PS) and power spectral density (PSD) for the determination of the frequency values of the spectrum and spectrum resonance spacing domains (SRSD). The experimental results presented here were obtained by the direct contact method using silicon gel as the coupling medium by pulse-echo technique. The instrumentation consisted of an IPR-100 pulser-receiver, a A/D-90 converter and a SMC-4 from Physical Acoustic Corporation, a sampler and a spectral analyzer. Keywords: ultrasounds, wavelets, power spectrum,power spectral density.