MM 12 Flüssige und amorphe Metalle III

Zeit: Freitag 14:45–16:15 Raum: TU H111

MM 12.1 Fr 14:45 TU H111

Diffusion in AlNiCe melts near the liquidus temperature — •Axel Griesche[1], Michael-Peter Macht[1], Rainer Schmid-Fetzer[2], and Günter Frohberg[3] — [1]Hahn-Meitner-Institute Berlin, Glienicker Str. 100, D-14109 Berlin — [2]Institute of Metallurgy, Technical University Clausthal, Robert-Koch-Straße 42, D-38678 Clausthal-Zellerfeld — [3]Institute of Material Sciences and Technology, Technical University Berlin, Hardenbergstr. 36, D-10623 Berlin

Interdiffusion and self diffusion in $Al_{87}Ni_{10}Ce_3$ and $Al_{77}Ni_{20}Ce_3$ melts were measured at 1273 K and 1373 K, respectively, using the long-capillary method. The chemical diffusion profiles were determined by means of energy dispersive x-ray spectroscopy (EDX). For self diffusion, the penetration profiles of stable ^{62}Ni and stable ^{142}Ce isotopes were measured by means of inductive-coupled plasma mass spectroscopy (ICP-MS). The thermodynamic factor was calculated from chemical potential data that were obtained by extrapolating the Gibbs free energy of the binary systems into the ternary melt using a Redlich-Kister model. The correlation between the interdiffusion coefficients, the self diffusion coefficients and the thermodynamic factor was studied by use of the Darken-Manning relation. The enhancement of chemical diffusion with respect to self diffusion correlates linearly with the thermodynamic factor.

MM 12.2 Fr 15:00 TU H111

Der Einfluss von Zusammensetzung und Struktur auf die atomare Diffusion in metallischen Flüssigkeiten — •Andreas Meyer — Physik Department E13, TU München

Wir untersuchen Struktur und Dynamik in Ni-P und Al-Ni Basislegierungen mit inelastischer Neutronenstreuung. In Ni, NiP, PdNiP und PdNiCuP Schmelzen hängen Liquidus und Unterkühlungseigenschaften stark von der Zusammensetzung ab. Die Diffusionskoeffizienten sind dagegen unabhängig von der Legierung: Der Massetransport ist dominiert von der Packungsdichte [1].

Al-Ni Legierungsschmelzen zeigen dagegen eine Nahordung auf intermediären Längenskalen. Diese geht einher mit einem stark nicht-lineraren Anstieg der Diffusionskoeffizienten mit steigendem Al Gehalt. In Kombination mit Molekulardynamik Simulationen zeigt sich, dass diese chemische Nahordnung die Ursache für eine nicht-lineare Abhängigkeit der Packungsdichte von der Zusammensetzung ist, die wiederum die atomare Diffusion kontrolliert.

[1] S. Mavila Chathoth, A. Meyer, M.M. Koza, F. Juranyi, Appl. Phys. Lett. (im Druck)

[2] S.K. Das, J. Horbach, M.M. Koza, S. Mavila Chathoth, A. Meyer, Appl. Phys. Lett. (eingereicht)

MM 12.3 Fr 15:15 TU H111

Structure and Dynamics of Amorphous Al-Ni Mixtures: Computer Simulations — •Subir K. Das, Jürgen Horbach, and Kurt Binder — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

A Monte Carlo (MC) and Molecular Dynamics (MD) computer simulation techniques are used to study the structure and dynamics of amorphous Al-Ni mixtures. The simulations are done at constant pressure ($p = 0$) to allow a direct comparison with experiments. As a model an embedded atom potential [1] is used. We elucidate the appearance of the prepeak in the experimental neutron scattering structure factor in Al-rich compositions [2]. Diffusion constants are computed as a function of composition and temperature. They show a good agreement with neutron scattering experiments [3] for different compositions and also for $Al_{80}Ni_{20}$ at different temperatures above 1000K (below that temperature crystallites are formed in the experiment whereas in the simulation the system can be supercooled). We study the dynamics of supercooled $Al_{80}Ni_{20}$ and analyze its properties by means of mode coupling theory. In particular, we show how the intermediate range order, as reflected by the aforementioned prepeak, affects the dynamics. Moreover, the validity of the Stokes-Einstein relation is checked.

[1] Mishin *et al.*, Phys. Rev. B **65**, 224114 (2002). [2] Maret *et al.*, Phys. Rev. B **42**, 1598 (1990). [3] S. K. Das, J. Horbach, M. M. Koza, S. Mavila Chatoth, A. Meyer, submitted to Appl. Phys. Lett.

MM 12.4 Fr 15:30 TU H111

Diffusion in a model metallic glass: heterogeneity and ageing — •Schober Herbert — IFF, Forschungszentrum Jülich

We report results of molecular dynamics simulations of a binary Lennard-Jones system at zero pressure in the undercooled liquid and glassy states. We first follow the evolution of diffusivity and dynamic heterogeneity with temperature and show their correlation. In a second step we follow the ageing of a quenched glass. As diffusivity decreases with ageing, heterogeneity increases. We conclude that the heterogeneity is a property of the inherent diffusion of the relaxed state. The variations with aging time can be explained by annealing of quenched defect structures. This annealing has the same decay constants for both diffusivity and heterogeneity of both components.

MM 12.5 Fr 15:45 TU H111

Modification of the crystallization sequence of amorphous Al$_{88}$Y$_7$Fe5 — •Nancy Boucharat, Harald Rösner, and Gerhard Wilde — Institute of Nanotechnology, Research Center Karlsruhe, P.O.B. 3640, D-76021 Karlsruhe, Germany

Al-rich glassy alloys have attracted extensive attention due to their thermal stability against crystallization, since upon heating a high number density of Al-nanocrystals can develop in a residual amorphous matrix. One of the intriguing challenges is the understanding of the kinetics involved in the crystallization process since the retention of high number densities of nanocrystals is not completely understood. Calorimetric and structural analyses of glassy $Al_{88}Y_7Fe_5$ have been performed after thermal treatments at temperatures well below the glass transition and after the incorporation of different immiscible elements, i.e. Pb and In into the melt prior to quenching. The results indicate clearly that the primary crystallization reaction can be markedly influenced with the addition of 1 at.% In or Pb. The impact of incorporated particles is examined on the basis of heterogeneous nucleation concepts that account for the microstructure changes. Additionally, it is shown that by modifying the concentration gradient that forms at the interface of growing Al-nanocrystals the nucleation of a new metastable ordered phase can be controlled. Support by the DFG is gratefully acknowledged.

MM 12.6 Fr 16:00 TU H111

TiNbCuNiAl nanocrystalline matrix composites with high strength and high elastic and plastic strain — •Uta Kühn, Nicolle Radtke, Annett Gebert, Norbert Mattern, and Ludwig Schultz — IFW Dresden, Institut für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany

High-strength Ti-Nb-Cu-Ni-Al alloys were prepared via arc melting and injection casting into a metal mold with dimensions of about 30 mm in diameter and 10 mm in height and 3 mm in diameter and 50 mm in length, respectively. The structure of the arc-melted ingots and as-cast samples was characterized by X-ray diffraction, optical microscopy, and transmission electron microscopy. Room-temperature compression tests were carried out with an electromechanical testing device under quasistatic loading. The structure of the Ti-based alloys consisted of a bcc b-Ti type phase and a small amount of an unknown nanocrystalline interdendritic phase as well. The optimization of the Ti-based alloy composition is performed to achieve both high strength and high ductility. Compression tests reveal that the composites undergo work hardening and plastic deformation prior to failure. The best combination of strength and ductility was found for a mold cast Ti-Nb-Cu-Ni-Al alloy, which presents a fracture strength of more than 2000 MPa coupled with a plastic strain of 24 These features significantly improve the mechanical behavior of such composites and opens the possibility of obtaining tailored mechanical properties by controlling composition and solidification conditions.