for the [0 1 0] direction of ξ'-Al-Pd-Mn. We have grown single crystals of orthorhombic $Al_{13}Co_4$using the Bridgman technique. In the as grown material defect analyses were performed by means of transmission electron microscopy.
The material contains planar defects terminated by dislocations. The planar defects were identified as stacking faults. By means of tilting series in the transmission electron microscope the plane normal of the faults was determined as parallel to the [0 0 1] lattice direction. We have performed two beam Bragg-contrast exit nction experiments and determined the strain-field direction of the planar faults and the terminating dislocations as parallel to the [3 2 0] direction. Hence we can conclude that partial-dislocation motion on (0 0 1) lattice planes by pure glide takes place in orthorhombic $Al_{13}Co_4$

MM 11.5 Fr 18:30 TU H1058

**Plastic deformation behaviour of $Al_{13}Co_4$ single crystals** — •Marc Heggen, Dewei Deng, and Michael Feuerbacher — Institut für Festkörperforschung Forschungszentrum Jülich GmbH, par 52425 Jülich, Germany

$Al_{13}Co_4$ is an orthorhombic phase with lattice parameters a = 0.82 nm, b = 1.24 nm, and c = 1.45 nm. It is a structurally complex alloy phase with 101 atoms per unit cell. The structural key feature of this material are pair-connected pentagonal prismatic channels along the b direction. Around these, the structure can be matched by alternatingly oriented flattened hexagons . $Al_{13}Co_4$ is a particularly interesting phase due to its structural relationship to ξ'-Al-Pd-Mn, in which the Metadislocation-mediated deformation process was discovered.
We have performed uniaxial deformation tests in compression on $Al_{13}Co_4$ single crystals, which were grown by means of the Bridgman technique. The material was deformed in a temperature range between 650 and 900 °C at strain rates of $10^{-5}$ and $10^{-4}$ $s^{-1}$. It shows pronounced yielding and continuous hardening after the lower yield point. Stress-relaxation tests, strain-rate changes and temperature-cycling tests were performed in order to determine thermodynamic activation parameters. The deformed samples show a number of slip lines on the surface oriented 45° with respect to the compression direction.

# 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 $Al_{88}Y_7Fe5$** — •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 modi-

fying 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.

## MM 13 Flüssige und amorphe Metalle IV

Zeit: Freitag 16:30–17:30 Raum: TU H111

MM 13.1 Fr 16:30 TU H111

**Shear-band propagation in fully amorphous and partially crystallised Mg-based alloys studied by nanoindentation and TEM** — •A. Castellero[1,2], S.J. Lloyd[1], Zs. Kovacs[3], S.V. Madge[1], M. Baricco[4], J.F. Löffler[2], and A.L. Greer[1] — [1]Dept. of Materials Science and Metallurgy, University of Cambridge, Cambridge, UK — [2]Lab. of Metal Physics and Technology, ETH Zurich, Zurich, Switzerland — [3]Dept. of General Physics, Eötvös Loránd University, Budapest, Hungary — [4]Dip. di Chimica IFM, Università di Torino, Torino, Italy

Initiation and propagation of discrete shear bands in metallic glasses can be observed as constant-load steps in the loading curve of nanoindentation measurements. For Mg60Cu30Y10 bulk metallic glass such steps, that can be easily observed in the as-quenched sample, have been found even in partially crystallised samples with a very high density of crystals (30-80 nm in diameter). Since such a grain size is comparable with the width of shear bands (10-60 nm) the band-propagation cannot be inhibited. TEM dark-field images show a variation in contrast to the amorphous phase in the region beneath the indent, suggesting the presence of medium-range order induced by relaxation. In the case of Mg66Ni20Nd14 the steps disappear for a crystalline fraction of about 50 percent and a grain size of 200 nm. Corresponding to a low density region around the indent tip, the indent profile becomes steeper suggesting that the material cannot recover elastically after the deformation. We propose that crystals larger than the width of a shear band are able to stop the bands originating from the indent tip, leading to a high concentration of free volume that cannot relax.

MM 13.2 Fr 16:45 TU H111

**Decomposition and Crystallization Behavior of Pd40Cu30Ni10P20 Bulk Metallic Glass** — •N. Wanderka, E. Davydov, and M.-P. Macht — Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany

The Pd40Cu30Ni10P20 glass is one of the most stable metallic bulk glasses. The main aim of this study was to investigate the crystallization pathway by differential scanning calorimetry , X-ray diffraction, transmission electron microscopy and by the three-dimensional atom probe. It is found that the glass decomposes in the supercooled liquid state before crystallization starts. The correlation between the decomposed amorphous phases and the primary crystalline phase of early crystallization stages is studied. The composition of the primary phase is similar to that of the crystalline phase which first forms during slow cooling of the liquid alloy melt. The chemical compositions of the different crystalline phases formed during slow cooling of the liquid melt as well as during annealing of the amorphous glass are analyzed and compared in the framework of the quasi ternary Pd-(Cu+Ni)-P system.

MM 13.3 Fr 17:00 TU H111

**Der Einfluß von La auf das Kristallisationsverhalten von amorphen $Al_{94-x}Ni_6La_x$ ($x = 4-7$) Legierungen** — •Markus Wollgarten[1], Kanai L. Sahoo[2,1], Jörg Haug[1] und John Banhart[1] — [1]Hahn-Meitner-Institut, Abt. Werkstoffe, Glienicker Str. 100, D-14109 Berlin — [2]National Metallurgical Laboratory, Jamshedpur-831007, India

Schmelzgesponnene und anschließend ausgelagerte Al-Legierungen mit einem Gehalt von 6 at.% Ni und 4 bis 7 at.% La wurden mit Differentialrasterkalorimetrie (DSC), Röntgendiffraktometrie, Kleinwinkelneutronenstreuung (SANS), Transmissionselektronenmikroskopie und Härtemessungen untersucht. Die Röntgendiffraktogramme zeigen, dass die Bänder in ihrem Ausgangszustand vollständig amorph sind, wohingegen die SANS-Daten auf Konzentrationsfluktuationen hindeuten. Die DSC-Experimente ergaben, dass die Kristallisation in zwei Schritten abläuft, wobei die Details der Kristallisationspfade vom La-Gehalt abhängig sind. SANS-Untersuchungen an ausgelagerten Proben lassen auf zwei unterschiedliche Ausscheidungsverteilungen schließen, die am Besten durch eine Kern-Hülle-Struktur erklärt werden können. Während des Auslagerungsprozesses wurden deutliche Änderungen der Mikrohärte beobachtet, die mit den Entwicklungsstufen der Mikrostruktur korreliert werden können.

MM 13.4 Fr 17:15 TU H111

**Widerstand, Thermokraft und Struktur amorpher $Al_{100-x}ÜM_x$-Legierungen** — •Jan Rauchhaupt, Uta Giegengack, Martin Stiehler und Peter Häussler — TU Chemnitz, 09107 Chemnitz

Amorphe Al-ÜM-Legierungen mit frühen ÜM (Sc, Ti, V, Cr) haben hochinteressante Eigenschaften bezüglich des elektronischen Transports, z.B. drastische Veränderungen des Temperaturkoeffizienten des Widerstand bei mittleren Temperaturen, Änderung des Vorzeichens der Thermokraft und sie sind sehr stabil. Wir stellen solche Legierungen in situ bei T= 4K unter HV-Bedingungen zunächst amorph her und tempern die Proben dann bis in den kristallinen Zustand. Es wird die statische Struktur durch Elektronenbeugung, der spezifische Widerstand und die Thermokraft jeweils als Funktion der Temperatur und der Zusammensetzung gemessen. Die Ergebnisse dieser Legierungen mit frühen ÜM sollen mit Vorhersagen eines allgemeineren Modells für späte Al-ÜM-Legierungen, welches durch Messungen der Legierungen $Al_{100-x}ÜM_x$ (ÜM = Mn, Fe, Co, Ni) bestätigt wurde, verglichen werden. Die Struktureigenschaften und das Transportverhalten werden als Ergebnis einer Resonanz zwischen dem Elektronensystem und der statischen Struktur mit Konsequenzen für die Phasenstabilität und den Transport diskutiert.