METALL- und MATERIALPHYSIK (MM)

Prof. Dr. Winfried Petry
Technische Universität München
Forschungs-Neutronenquelle FRM II und Physik Department E13
D-85747 Garching
E-Mail: wpetry@frm2.tum.de

ÜBERSICHT DER HAUPTVORTRÄGE UND FACHSITZUNGEN

(Hörsäle TU H111, TU H1058, TU H2038)

Hauptvorträge

MM 1.1	Fr	09:45	(TU H1058)	**Exchange coupled magnetostrictive multilayers**, Eckhard Quandt
MM 5.1	Fr	10:30	(TU H1058)	**The world of complex metallic compounds and the CMA European Network of Excellence**, Jean-Marie Dubois, Louis Schlapbach, Knut Urban
MM 7.1	Fr	14:00	(TU H1058)	**Colloidal Particles - a 3-D Analogue Computer for Materials Research**, Peter Schall, David A. Weitz, Frans Spaepen
MM 8.1	Fr	14:45	(TU H1058)	**Electronic structure of Frank-Kasper Al-Mg based compounds**, Esther Belin-Ferré
MM 10.1	Fr	17:00	(TU H1058)	**Magnetic and Transport Properties of Al-based Complex Metallic Alloys**, Janez Dolinsek
MM 15.1	Sa	08:30	(TU H1058)	**Modelling of phase transformations : from the lab to the plant**, Yves J.M. Bréchet
MM 22.1	Sa	14:00	(TU H1058)	**Engineering Materials Research with Neutrons and Photons: Contributions to better Lightweight Structures**, Andreas Schreyer
MM 26.1	Mo	09:45	(TU H1058)	**Size effects in metal plasticity**, Cynthia A. Volkert
MM 29.1	Mo	10:30	(TU H1058)	**Nanoscale electron tomography for materials science**, P.A. Midgley, T.J.V. Yates, J.R. Tong, I. Arslan
MM 31.1	Mo	14:00	(TU H1058)	**Finite temperature ab initio modeling of formation and migration of impurities, point defects and planar faults** , Walter Wolf
MM 33.1	Mo	16:30	(TU H1058)	**New trends in synchrotron-based tomography**, Cloetens P.
MM 35.1	Di	09:45	(TU H1058)	**Prediction of material fatigue**, Karl Maier
MM 36.1	Di	10:30	(TU H1058)	**Synchrotron X-ray microtomography: principles and applications**, A. Haibel, A. Rack, S. Zabler, J. Banhart
MM 42.1	Di	14:00	(TU H1058)	**Atomic size matters**, Mike Finnis
MM 43.1	Di	14:45	(TU H1058)	**Absorption- and phase-based imaging signals for neutron tomography**, Wolfgang Treimer
MM 45.1	Di	16:30	(TU H1058)	**Neutron tomography as tool for applied research and technical inspection**, Eberhard H. Lehmann, Peter Vontobel

Fachsitzungen

MM 1	**Hauptvortrag Eckhard Quandt**	Fr 09:45–10:15	TU H1058	MM 1.1–1.1
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MM 3	**Flüssige und amorphe Metalle II**	Fr 11:30–12:30	TU H111	MM 3.1–3.4
MM 4	**Wasserstoff in Metallen**	Fr 10:30–12:00	TU H2038	MM 4.1–4.6
MM 5	**Symposium Complex Metallic Alloys, Hauptvortrag Jean-Marie Dubois**	Fr 10:30–11:00	TU H1058	MM 5.1–5.1
MM 6	**Symposium Complex Metallic Alloys I**	Fr 11:00–12:15	TU H1058	MM 6.1–6.5
MM 7	**Hauptvortrag Peter Schall**	Fr 14:00–14:30	TU H1058	MM 7.1–7.1

MM 8	**Symposium Complex Metallic Alloys, Hauptvortrag Esther Belin-Ferré**	Fr	14:45–15:15	TU H1058	MM 8.1–8.1
MM 9	**Symposium Complex Metallic Alloys II**	Fr	15:15–16:30	TU H1058	MM 9.1–9.5
MM 10	**Symposium Complex Metallic Alloys, Hauptvortrag Janez Dolinsek**	Fr	17:00–17:30	TU H1058	MM 10.1–10.1
MM 11	**Symposium Complex Metallic Alloys III**	Fr	17:30–18:45	TU H1058	MM 11.1–11.5
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MM 13	**Flüssige und amorphe Metalle IV**	Fr	16:30–17:30	TU H111	MM 13.1–13.4
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MM 15	**Hauptvortrag Yves Bréchet**	Sa	08:30–09:00	TU H1058	MM 15.1–15.1
MM 16	**Phasenumwandlung I**	Sa	09:15–10:45	TU H1058	MM 16.1–16.6
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MM 18	**Nanoskalige Materialien I**	Sa	09:15–10:45	TU H111	MM 18.1–18.6
MM 19	**Nanoskalige Materialien II**	Sa	11:00–12:30	TU H111	MM 19.1–19.6
MM 20	**Intermetallische Phasen I**	Sa	09:15–10:30	TU H2038	MM 20.1–20.5
MM 21	**Intermetallische Phasen II**	Sa	11:00–12:15	TU H2038	MM 21.1–21.5
MM 22	**Hauptvortrag Andreas Schreyer**	Sa	14:00–14:30	TU H1058	MM 22.1–22.1
MM 23	**Phasenumwandlung III**	Sa	14:45–16:30	TU H1058	MM 23.1–23.7
MM 24	**Nanoskalige Materialien III**	Sa	14:45–16:00	TU H111	MM 24.1–24.5
MM 25	**Material Design**	Sa	14:45–16:30	TU H2038	MM 25.1–25.7
MM 26	**Hauptvortrag Cynthia Volkert**	Mo	09:45–10:15	TU H1058	MM 26.1–26.1
MM 27	**Quasikristalle**	Mo	10:30–11:45	TU H111	MM 27.1–27.5
MM 28	**Elektronische Eigenschaften**	Mo	10:30–12:00	TU H2038	MM 28.1–28.6
MM 29	**Symposium Tomographic Methods in Materials Research Hauptvortrag Paul Midgley**	Mo	10:30–11:00	TU H1058	MM 29.1–29.1
MM 30	**Symposium Tomographic Methods in Materials Research**	Mo	11:00–12:40	TU H1058	MM 30.1–30.5
MM 31	**Hauptvortrag Walter Wolf**	Mo	14:00–14:30	TU H1058	MM 31.1–31.1
MM 32	**Poster TU B (Symposium Tomographic Methods in Materials Research M-32.32-55)**	Mo	14:30–16:30	Poster TU B	MM 32.1–32.54
MM 33	**Symposium Tomographic Methods in Materials Research Hauptvortrag Cloetens**	Mo	16:30–17:00	TU H1058	MM 33.1–33.1
MM 34	**Symposium Tomographic Methods in Materials Research**	Mo	17:00–18:00	TU H1058	MM 34.1–34.3
MM 35	**Hauptvortrag Karl Maier**	Di	09:45–10:15	TU H1058	MM 35.1–35.1
MM 36	**Symposium Tomographic Methods in Materials Research Hauptvortrag Astrid Haibel**	Di	10:30–11:00	TU H1058	MM 36.1–36.1
MM 37	**Symposium Tomographic Methods in Materials Research**	Di	11:00–12:40	TU H1058	MM 37.1–37.5
MM 38	**Mechanische Eigenschaften I**	Di	10:30–11:30	TU H111	MM 38.1–38.4
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MM 40	**Diffusion I**	Di	10:30–11:30	TU H2038	MM 40.1–40.4
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MM 42	**Hauptvortrag Mike Finnis (Max-Born Preisträger)**	Di	14:00–14:30	TU H1058	MM 42.1–42.1
MM 43	**Symposium Tomographic Methods in Materials Research Hauptvortrag Wolfgang Treimer**	Di	14:45–15:15	TU H1058	MM 43.1–43.1
MM 44	**Symposium Tomographic Methods in Materials Research**	Di	15:15–16:15	TU H1058	MM 44.1–44.3
MM 45	**Symposium Tomographic Methods in Materials Research Hauptvortrag Eberhard Lehmann**	Di	16:30–17:00	TU H1058	MM 45.1–45.1
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MM 47	**Mechanische Eigenschaften III**	Di	14:45–16:00	TU H111	MM 47.1–47.5
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MM 49	**Grenzflächen I**	Di	14:45–16:00	TU H2038	MM 49.1–49.5
MM 50	**Grenzflächen II**	Di	16:30–17:45	TU H2038	MM 50.1–50.5

Mitgliederversammlung des Fachverbands Metall- und Materialphysik

Di 18:00–19:00 TU H2038

Tagesordnung

Berichte des Fachverbandsvorsitzenden und des AGM Vorsitzenden

Frühjahrstagung 2005, Beiträge, Statistiken

Frühjahrstagung 2006 in Dresden gemeinsam mit der EPS

Neue Themenfelder und Symposia für die Metall- und Materialphysik

Vorschläge für Hauptvorträge

Sonstiges

Fachsitzungen

– Haupt-, Kurzvorträge und Posterbeiträge –

MM 1 Hauptvortrag Eckhard Quandt

Zeit: Freitag 09:45–10:15 Raum: TU H1058

Hauptvortrag MM 1.1 Fr 09:45 TU H1058

Exchange coupled magnetostrictive multilayers — •Eckhard Quandt — Center of Advanced European Studies and Research (caesar), Bonn

Sputter-deposited giant magnetostrictive thin films present an interesting approach to realize novel sensors or actuators as they offer features like contactless, high frequency operation, simple actuator designs and a cost-effective manufacturing technique. Essential for these applications was the development of exchange coupled multilayers showing low field giant magnetostriction. Particularly, multilayers consisting of amorphous giant magnetostrictive Tb-Fe layers with positive magnetostriction and nanocrystalline soft magnetic Fe-Co layers having a very high magnetization present a type of a spring-magnet-type system which shows very high magnetoelastic energies at very low fields [1]. The saturation field of these multilayers can be considerably reduced compared to single layer materials due to the increased magnetization and the reduced anisotropy while keeping relatively large values of the magnetostriction. In general, applications of these materials require a well-defined uniaxial in-plane anisotropy, which e.g. can be obtained by annealing under a magnetic field. Further materials development issues of these giant magnetostrictive multilayers will be discussed in view of a possible use as a very sensitive magnetic field sensor [2].

[1] Quandt, E.; Ludwig, A.: J. Appl. Phys. 85 (1999) 6232-37. [2] Stein, S.; Wuttig, M.; Viehland, D.; Quandt, E.: J. Appl. Phys., 2004 (in press).

MM 2 Flüssige und amorphe Metalle I

Zeit: Freitag 10:30–11:30 Raum: TU H111

MM 2.1 Fr 10:30 TU H111

Electrochemistry and biocompatibility of Zr-based Bulk Metallic Glasses — •Stefano Buzzi[1], Kaifeng Jin[1], Samuele Tosatti[2], Isabel Gerber[3], Peter J. Uggowitzer[1], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, ETH Zürich, 8093 Zürich, Switzerland — [2]Biomedical Interfaces Team, Laboratory for Surface Science and Technology, ETH Zürich, Switzerland — [3]Institute of Cell Biology, ETH Zürich, Switzerland

Bulk metallic glasses are promising materials for medical applications because of their high strength and elasticity. In order to determine their biocompatibility as a function of sample preparation, a selected group of these materials was characterized by XPS and electrochemical methods (potentiodynamic measurements and solution analysis). Their cytotoxicity was also analyzed by measuring the viability and metabolic activity of a mouse fibroblast cell line. The results indicate that pitting corrosion takes place in the presence of chloride-ion concentrations comparable to body conditions. Furthermore, it was shown that plasma treatment stabilizes the natural ZrO2 adlayer, and that the cells are able to grow on the Zr-based glasses with good viability and metabolic activity. Among the Zr-based alloys, the most metabolic activity was observed in a Ni-free alloy developed by our group. In contrast, the cells cultured on the Cu-Ti-based metallic glasses hardly grew at all.

MM 2.2 Fr 10:45 TU H111

Reversible formation and disappearance of free volumes in a bulk metallic glass — F. Ye[1,2], •W. Sprengel[1], R.K. Wunderlich[3], H.-J. Fecht[3], H. Dosch[2], and H.-E. Schaefer[1] — [1]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, Stuttgart, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [3]Universität Ulm, Materials Division, Ulm, Germany

In the bulk metallic glass $Zr_{57}Cu_{15.4}Ni_{12.8}Nb_5Al_{10}$ the reversible formation and disappearance of free volumes have been detected by time-differential dilatometry studies in analogy to the observation of thermal vacancy formation in B2-intermetallics (H.-E. Schaefer et al., PRL **82**, 948 (1999)). After an initial long-term annealing of the bulk amorphous system at 593 K cycles of fast temperature changes have been carried out below the glass temperature $T_g = 672$ K and subsequent time-dependent reversible elongation after fast heating or shrinking after fast cooling has been observed by isothermal interferometric dilatometry. During these processes no changes of the amorphous structure were detected. This demonstrates that free volumes are reversibly formed or disappear in a deeply metastable structure. The kinetics of the time-dependent process indicate that an entire ensemble of atoms is involved in the thermal formation of free volumes in the bulk amorphous solid.

MM 2.3 Fr 11:00 TU H111

Bulk Metallic Glass Formation in ZrCuFeAl alloys — •K.F. Jin and J. F. Löffler — Laboratory of Metal Physics and Technology, ETH Zürich, 8093 Zürich, Switzerland

We present a series of Ni-free Zr-based bulk metallic glasses where the critical casting thickness (in rod-shape) reaches values of up to 13 mm in diameter. The glass-forming region of this family of alloys is very extensive, and nearly 15 percent of their Zr or Cu content may be varied while still maintaining a critical casting thickness of 1 mm. The alloys were investigated via x-ray diffraction (XRD), small-angle neutron scattering (SANS) and differential scanning calorimetry (DSC). XRD and SANS confirm a glassy structure, while DSC determines a calorimetric glass transition between 665 K and 687 K and an undercooled liquid region extending up to 86 K. Mechanical tests performed on the glassy alloys reveal a tensile yield strength of 1.7 GPa and an elastic limit of 2.25 percent. In addition, crystallization studies show the formation of a nanometer-sized icosahedral phase with a quasilattice constant of 4.76 angstrom. The superior properties of these bulk metallic glasses, their glassy structure and the fact that they are Ni free, make them interesting candidates for biomedical applications.

Supported by ESM (Entwicklungsfonds Seltene Metalle)

MM 2.4 Fr 11:15 TU H111

Transformations near the glass transition in Pd-based bulk metallic glasses — •Shantanu V. Madge, Harald Rösner, and Gerhard Wilde — Institute of Nanotechnology, Forschungszentrum Karlsruhe, P.O.B. 3640, D-76021 Germany.

One reason for the current interest in bulk metallic glasses (BMGs) is the complexity that often underlies crystallisation in these alloys, which can involve various metastable phases. Phase separation in the undercooled liquid is an issue that has seen much attention in recent years in order to explain the counter-intuitive nanocrystallisation that occurs in some BMGs. In the present work, a series of Pd-based BMGs has been prepared by suction-casting. The transformations in certain glasses on heating above the glass-transition temperature are investigated $in-situ$ and $ex-situ$ by complementary techniques such as modulated-temperature calorimetry, X-ray diffraction or transmission electron microscopy, including the analysis of the initial crystallization products in the early stages of devitrification. The results are discussed in the light of possible amorphous phase separation that has been suggested to occur in many BMGs including some Pd-rich systems.

MM 3 Flüssige und amorphe Metalle II

Zeit: Freitag 11:30–12:30 Raum: TU H111

MM 3.1 Fr 11:30 TU H111

Untersuchung magnetischer und mikrostruktureller Eigenschaften der massiven glasbildenden Legierung $Nd_{60}Fe_{30}Al_{10}$ — •A. Bracchi[1], K. Samwer[2], T. Niermann[1], M. Seibt[1] und S. Schneider[1] — [1]IV. Physikalisches Institut, Universität Göttingen, 37077 Göttingen — [2]I. Physikalisches Institut, Universität Göttingen, 37077 Göttingen

Massive glasbildende $Nd_{60}Fe_{30}Al_{10}$ Proben, die mit einer Abkühlrate von 100 K/s aus der Schmelze hergestellt wurden, sind mit SQUID-Magnetometrie, Kleinwinkelneutronenstreuung (SANS) und hochenergetischer Röntgenbeugung charakterisiert worden. Die SQUID-Messungen im Temperaturbereich von 4.2 K bis 650 K zeigen zwei Übergänge, die auf zwei magnetische Phasen hinweisen. Die magnetischen Eigenschaften lassen sich in dem Temperaturbereich (50 K < T < 470 K), in dem nur eine ferromagnetische Phase vorliegt, mit dem „Domain-Wall-Pinning“ Modell deuten. Um die Mikrostruktur der Probe und die „Pinning“ Zentren zu charakterisieren, wurden SANS Messungen mit polarisierten und nicht polarisierten Neutronen durchgeführt. Aus diesen Messungen wurden strukturelle und magnetische charakteristische Längen ermittelt. Zur Deutung der magnetischen Eigenschaften und der Streuergebnisse wird ein paramagnetic core-ferromagnetic shell model für nanokristalline Ausscheidungen in einer ferromagnetischen amorphen Matrix vorgeschlagen.

Dieses Projekt wird von der DFG in Rahmen des SFB 602 gefördert.

MM 3.2 Fr 11:45 TU H111

Mechanical properties of slowly cooled Zr-based composites containing dendritic bcc phase precipitates — •Nicolle Radtke[1], Jürgen Eckert[1,2], Uta Kühn[1], and Ludwig Schultz[1] — [1]IFW Dresden, Institut für Metallische Werkstoffe, Postfach 270016, 01171 Dresden — [2]TU Darmstadt, Institut für Physikalische Metallkunde, Petersenstr. 23, 64287 Darmstadt

We report about the microstructure, thermal stability and the mechanical properties of slowly cooled Zr-Nb-Cu-Ni-Al alloys with ductile bcc phase precipitates embedded in a glassy or a nanocrystalline matrix. The samples were prepared in form of rods by injection casting into a copper mould. The phase formation and the microstructure of the composite material are investigated by X-ray diffraction, EDX-analysis, scanning and transmission electron microscopy. The thermal stability was examined by differential scanning calorimetry and the mechanical behaviour was investigated by compression tests under quasistatic loading at room temperature and at higher temperatures. The formation of bcc phase dendrites and a glassy or a nanocrystalline matrix is strongly governed by the alloy composition and the actual cooling rate during solidification. Besides, changes in composition and cooling rate lead to different volume fraction and size of the bcc phase precipitates and, hence, to different values of yield strength, elastic and plastic strain. The formation of a nanocrystalline matrix depends on the melting temperature of the alloy and, hence, the cooling rate. Surprisingly, these sample exhibits higher yield strength and plastic strain than the samples containing an amorphous matrix.

MM 3.3 Fr 12:00 TU H111

The temperature dependence of the deGennes narrowing in liquid Rubidium — •Franz Demmel[1] and Christoph Morkel[2] — [1]ILL, Grenoble — [2]TU München, München

Recent diffraction experiments on levitated undercooled liquid metals have been modelled with a contribution of icosahedral clusters in the melt. The temperature dependence of the density time correlation function at next neighbour distances should also be a sensitive parameter for detecting clusters and their possible melting. We performed coherent inelastic neutron scattering experiments on the alkali metal Rubidium around the structure factor maximum. Fifteen temperatures from the melting point up to two times the melting point have been measured. The experiment was performed at three axis spectrometers of the Forschungsreaktor München FRM and at the ILL, Grenoble. The line width shows a linear increase with temperature. But the peak values decrease in a nonlinear way and indicate a change in dynamics around $1.5*T_{melt}$. One can speculate whether this decrease in amplitude above the macroscopic melting temperature is related to the melting of solid-like structures (clusters) in the liquid state.

MM 3.4 Fr 12:15 TU H111

Diffraction Studies On the Short-Range Order in Metallic Melts — •Dirk Holland-Moritz[1], Thomas Schenk[1], Oliver Heinen[1], Virginie Simonet[2], Robert Bellissent[3], and Dieter M. Herlach[1] — [1]DLR, Institut für Raumsimulation, D-51147 Köln — [2]Laboratoire Louis Néel, CNRS, BP166, F-38042 Grenoble Cedex 9 — [3]Centre d'Études Nucléaires de Grenoble, DRFMC/SPSMS/MDN, F-38054 Grenoble Cedex

Following the pioneering work of Frank, an icosahedral short-range order should be energetically favoured in undercooled metallic melts. This hypothesis was recently experimentally confirmed by neutron- and X-ray diffraction investigations on stable and undercooled liquids of the pure metals Ni, Co, Zr and Fe and of various alloys forming quasicrystals and polytetrahedral phases. In this work we present experiments on the short-range order of undercooled $Co_{75}Pd_{25}$ melts. These melts are of special interest because they show the onset of magnetic ordering if they are undercooled close to the magnetic Curie temperature. Moreover, investigations on the short-range order of stable and undercooled melts of Ti are presented. The liquids were containerlessly processed und undercooled by use of the electromagnetic levitation technique which was combined with the technique of energy dispersive diffraction of synchrotron radiation and elastic neutron scattering in order to determine the structure factors. For both sample materials, similar as for most other metallic melts, the measured structure factors are well described if an icosahedral short-range order is assumed to prevail in the melt. This work was supported by DFG under contract Nos. Ho1942/1, Ho1942/2 and Ho1942/4.

MM 4 Wasserstoff in Metallen

Zeit: Freitag 10:30–12:00 Raum: TU H2038

MM 4.1 Fr 10:30 TU H2038

Mesopore Formation in FeAl Ribbons by Supersaturated Vacancies Clustering for hydrogenation studies — •Tomohide Haraguchi[1,2], Astrid Pundt[1], Reiner Kirchheim[1], Hitoshi Hashimoto[2], Kyosuke Yoshimi[3], and Shuji Hanada[3] — [1]Institut für Materialphisik der Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Research Institute for Sustainable Development, National Institute of Advanced Industrial Science and Technology, Nagoya 463-8560, Japan — [3]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Many researchers have focused their research on the surface rich materials like zeolites, carbon-related materials, foams and so on. We present the mesopore formation on the surface of rapidly solidified FeAl alloy ribbons. The pores are observed after annealing at definite temperature and are caused by the clustering of the supersaturated thermal vacancies during the relaxation process. The size of pores is several tens nm, this being much smaller than that of porous metallic materials such as foamed, sponge-like and sintered metals. Once a large number of mesopores are formed on the surface, specific surface area would increase drastically. Effect of mesopores on the hydrogen absorption process is also planed to be presented.

MM 4.2 Fr 10:45 TU H2038

Hydrogen absorption of Na-Li alanates prepared by ball-milling — •RYOTA GEMMA[1], HARU-HISA UCHIDA[1], ASTRID PUNDT[2], and REINER KIRCHHEIM[2] — [1]Dept. of Human Development, Tokai University, 259-1292, Kitakaname, Hiratsuka, Kanagawa, Japan — [2]Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077, Göttingen, Germany

In recent years, complex hydrides based on Na, Li and Al have been of interest for hydrogen storage because of their high hydrogen capacity

at around 3-5wt%. In this study Na_2LiAlH_6 prepared by ball-milling was investigated by determining its P-C-T property which has not been well introduced up to now. The extrapolation of the vant Hoff plot of plateau pressures showed the possibility of reversible sorption reaction at around room temperature. But, the high apparent activation energy of 110-130 $kJ/molH_2$ in the absorption was found to be appropriate for middle temperature use. An appropriate mixing of rare-earth oxides powder in the course of milling enhanced the reaction rate. This was interpreted by increased specific surface by finely dispersed oxides.

MM 4.3 Fr 11:00 TU H2038

Characterization of the dehydrogenation of alanates with different catalyst monitored by proton NMR — •Laura Esther Valiente-Banuet, Eva Stanik, and Günter Majer — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

$NaAlH_4$ is a promising material for the development of reversible hydrogen storage systems. The kind of pre-treatment of the material and the catalyst play a crucial role in the increase of the de- and re-hydriding rates. This also influences the reduction in the temperature of dehydrogenation. However, the microscopic mechanism and the change of the hydrogen mobility due to the catalyst are not yet completely understood. In this work we report on NMR studies of the hydrogen desorption from $NaAlH_4$ doped with the catalysts $TiCl_3$ and Ti_{13}-clusters, respectively. The time dependence of the NMR spectra, measured at a given temperature, shows clearly the transition from $NaAlH_4$ to Na_3AlH_6. The hydrogen dynamics in the different compounds is investigated by measurements of the spin-lattice relaxation. In the case of $NaAlH_4$ a double-exponential recovery of the nuclear magnetization is observed, which indicates two fractions of hydrogen with different mobilities.

MM 4.4 Fr 11:15 TU H2038

Lattice distortions in β-$YH_{2+\delta}$ and cubic YH_3 thin films studied by Raman spectroscopy. — •A.-M. Racu[1], M. Rode[1], D. Zur[1], A. Borgschulte[2], R. Westerwaal[2], and J. Schoenes[1] — [1]Institut für Halbleiterphysik und Optik, TU Braunschweig, Mendelssohnstrasse 3, 38106 Braunschweig, Germany — [2]Division of Physics and Astronomy, Faculty of Sciences, Vrije Universiteit, De Boelelaan 1081, Amsterdam, The Netherlands

We have monitored with Raman spectroscopy the metal insulator transition of Y films grown on (111) CaF_2 substrates and capped with Pd. The γ phase (YH_3) has a hexagonal structure characterized by a Raman spectrum with nine lines at room temperature. The stoichiometric β phase (YH_2) is cubic and shows only one line. In the superstoichiometric β phase of $YH_{2+\delta}$ we find changes in the spectra which are not compatible with a cubic lattice. There are clear indications that the cubic lattice is distorted into a tetragonal structure in $YH_{2+\delta}$. The Raman mapping image during unloading of an Y film shows a regime of coexistence between the γ and the superstoichiometric β phase. The results are compared with measurements on $Mg_zY_{1-z}H_x$ which also show a distortion of the cubic lattice.

MM 4.5 Fr 11:30 TU H2038

Ortsaufgelöste thermische Wasserstoffdesorption aus dem Volumen — •Martin Hövel, Matz Haaks und Karl Maier — Helmholtz - Institut für Strahlen- und Kernphysik der rheinischen Friederich-Wilhelms Universität zu Bonn

Die im Flugzeugbau verwendete schweißbare Aluminiumlegierung (AA6013) zeigt, gegenüber der traditionellen Legierung (AA2024), bei einer zyklischen Belastung in korrosiven Medien eine erhöhte Rissausbreitungsgeschwindigkeit, sowie ein langsameres Ausheilen von Punktdefekten in der plastischen Zone. Verantwortlich für dieses Verhalten ist wahrscheinlich der während der Rissentstehung in das Zwischengitter eindiffuniderende Wasserstoff.

Standardmethoden sind für den Nachweis dieser geringen Wasserstoff-Konzentration nicht geeignet.

Die bewährte Methode der thermischen Wasserstoffdesorption wurde weiterentwickelt, um ortsaufgelöst Wasserstoff im Volumen nachzuweisen. Dabei wird die Probe im Hochvakuum (HV) so eingesägt, dass die Späne unmittelbar in einen beheizten Tiegel im darunterliegende Ultrahochvakuum (UHV) Bereich fallen. Der Wasserstoff, der dabei aus den erhitzten Spänen ausdiffunidert, kann über die Druckerhöhung im UHV nachgewiesen werden.

MM 4.6 Fr 11:45 TU H2038

Hydrogen absorption in polymer and surfactant stabilised clusters — •M. Suleiman, J. Faupel, C. Borchers, H. U. Krebs, R. Kirchheim, and A. Pundt — Institute fuer Materialphysik, Univ. Goettingen

In this work the H-absorption behaviour in Pd clusters stabilised in two different matrix, polymer ((hard matrix)) and surfactant ((soft matrix)), will be presented. The effect of the stabiliser type and hence the morphology of the sample on the hydrogen uptake will be studied. Pressure-lattice parameter isotherms, obtained from in situ XRD measurements, were constructed for three samples: surfactant stabilised clusters, and two types of polymer stabilised samples ((clusters and closed clusters layers sample)). The pressure-lattice parameter isotherms for the samples show a narrowed lattice parameter miscibility gap [[1]]. The closed clusters layers sample shows the smallest lattice parameter expansion values. The effect of the samples morphology on the lattice expansion and the plateau slope will be discussed. It will be shown that not only the sample sizes affect the expansion but also the cluster surrounding plays an important rule.

This work is supported by the DPG via SEB 602

[[1]] M.Suleiman, J. Faupel, C. Borchers, H. U. Krebs, R. Kirchheim, A. Pundt submiited to JALCOM

MM 5 Symposium Complex Metallic Alloys, Hauptvortrag Jean-Marie Dubois

Zeit: Freitag 10:30–11:00 Raum: TU H1058

Hauptvortrag

MM 5.1 Fr 10:30 TU H1058

The world of complex metallic compounds and the CMA European Network of Excellence — •Jean-Marie Dubois[1], Louis Schlapbach[2], and Knut Urban[3] — [1]Ecole des Mines, Parc de Saurupt, F-54042 Nancy — [2]EMPA, CH-8600 Zürich — [3]Forschungszentrum Jülich GmbH, D-52425 Jülich

Complex Metallic Alloys encompass a broad variety of compounds and phases that are characterized by i) large unit cells, comprising tens up to thousands of atoms, ii) the presence of well-defined atom clusters, most often of icosahedral point group symmetry, iii) the occurrence of disorder in the ideal structure. As a result, most physical properties show distinct differences with respect to the behaviour of normal metallic alloys and therefore these materials possess a high potential for application in technology. With the support of about sixty industrial companies, the CMA European Network of Excellence contributes to a strengthening of the competitiveness of metallic materials for the benefit of European industries by the formation of a European Network of Excellence CMA. The Network unites 19 high-reputation core-group members, representing a person-year critical mass of 253 p.y and 84 Ph.D. students in 12 countries. On this basis, the project is designed to strengthen the competitiveness of European industries wherever materials need to offer hybrid properties, being both structural and functional, or embody an extraordinary combination of properties that are mutually excluding in conventional materials.

MM 6 Symposium Complex Metallic Alloys I

Zeit: Freitag 11:00–12:15 Raum: TU H1058

MM 6.1 Fr 11:00 TU H1058

Syntesis and crystal growth of Complex Metallic Alloys (CMA) — •Wolf Assmus[1], Stefan Brühne[1], Michael Feuerbacher[2], Guido Kreiner[3], and Eckhard Uhrig[1] — [1]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Robert-Mayer-Str. 2-4, D-60054 Frankfurt am Main — [2]Institut für Mikrostrukturforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich — [3]MPI für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, D-01187 Dresden

In the Virtual Integrated Laboratory A (VIL A – Materials Design and Synthesis) a number of european labs are working in a NoE on materials design, synthesis and crystal growth of CMA. All methods which are necessary for this research field as e.g. DTA, EMPA, X-ray analysis; especially for materials preparation and crystal growth techniques as arc-melting, melt-spinning, zone-melting, Czochralski, Bridgman or flux growth are available. Some examples of recent research in VIL A are discussed: Icosahedral and periodic Mg-Zn-*RE* alloys and a variety of periodic, huge unit cell Mg-Zn, Al-Pd, Al-Mg and related ternary CMA have been grown. For the growth of such complex alloys information about the phase-diagram must be available. It is important to know whether the phase is formed by direct cooling of the melt (congruent melting behaviour) or by peritectic or peritectoidic reaction. As another example in the Mg-Pd system it is shown that the phase width of Mg_6Pd (cF396) can be well understood from correlated disorder of only two atom sites in the $a \approx 2$ nm cubic unit cell.

MM 6.2 Fr 11:15 TU H1058

Structure-Property Relationships of Complex Intermetallic Phases — •Walter Steurer — Laboratory of Crystallography, Department of Materials, ETH Zurich, CH-8093 Zurich, Switzerland

It is amazing how sensitive some physical properties are to slight variations in the chemical composition of a complex intermetallic phase and its thermal history. Experiments on the most complex intermetallic phases, the quasicrystals, have shown that even annealing times of several thousand hours at two third of the melting temperature may be not sufficient to reach the equilibrium state. Non-equilibrium defects such as dislocations and nanodomain structures as well as chemical disorder may locally break the symmetry. In particular, cluster-based structures with a high-degree of pseudosymmetry tend to form orientationally twinned domain structures with rather low interfacial energy.

Materials creation and design crucially depends on materials characterization. Measurements of physical properties are only meaningful if they are reproducible. The results can only be reasonably interpreted and contribute to the understanding of a material if its chemical composition, crystal and defect structure are accurately known. On a few examples, the importance of materials analysis as function of composition, temperature and pressure is demonstrated.

MM 6.3 Fr 11:30 TU H1058

VIL C: Physical properties of complex metallic alloys — •Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The physical properties of complex metallic alloys are dominated by the interplay of two length scales: that of the local coordination polyhedra and that of the lattice constants. Expressed differently, a long range translational order is competing with a short range disorder. The consequences are, for example, backfolded energy bands which together with disorder induced scattering inhibit electronic and heat transport. Anharmonic flip motions are coupled to harmonic modes. Alternative atomic and cluster positions allow structural rearrangements and lead to new plastic modes and stress-induced phase transitions. The Virtual Integrated Laboratory C of the NoE-CMA will investigate these properties theoretically and experimentally within three workpages. A report will be given on state of the art, methods, and expectations.

MM 6.4 Fr 11:45 TU H1058

Surface physics, chemistry and nanoscience of complex metallic alloys — •Ronan McGrath[1], Marie-Geneviève Barthés-Labrousse[2], Karsten Horn[3], and Guy Tréglia[4] — [1]Dept. of Physics, the University of Liverpool, UK — [2]CNRS Vitry, France — [3]Fritz-Haber Institute, Berlin, Germany — [4]CNRS Marseilles, France

The surface physics, chemistry and nanoscience of complex metallic alloys (CMAs) presents many new challenges. For many existing experimental and theoretical techniques, the investigation of the large unit cell periodic alloys are on the borderline of what is feasible, especially with quantitative structural probes. It seems likely that many of the modifications of these techniques developed for the study of the aperiodic quasicrystal surfaces will be useful for these materials. The scientific study of these materials will break new ground, and the work will focus on three areas. The first is the understanding of the clean surface structure and properties of representative CMAs. Here there is especial interest in the study of the electronic structure close to the Fermi edge to compare with studies on related simple metal and quasicrystal phases. The second area is the investigation of the use of these surfaces as templates for the formation of low dimensional nanostructures, i.e. quantum dots and ultra-thin films. and of particular interest is how the cluster sub-structure will influence growth mechanisms for these materials. The third area of interest is the investigation of the properties of these materials in ambient environments. The results of these studies will form a crucial input to the design of potential devices based on CMAs.

MM 6.5 Fr 12:00 TU H1058

Advanced technologies for the preparation of coatings containing complex metallic alloys — •Constantin Vahlas[1] and Witold Gulbinski[2] — [1]Centre Interuniversitaire de Recherche et d Ingenierie des Materiaux (CIRIMAT-CNRS), Toulouse, France — [2]Physics Department, Faculty of Mechanical Engineering, Technical University of Koszalin, Poland

The development of advanced technologies for the processing of CMA-based coatings presents a major interest for numerous application domains. Indeed such technologies are widely recognized to be key underpinning and critically enabling areas of R&D on which most industrial sectors and fields of technology application, directly or indirectly depend. The presentation will introduce the state of the art in this field and the projected research within the CMA Network of Excellence. The use of selected PVD and MOCVD techniques will allow for processes and materials optimization with regard to the aimed application (e.g. hard and/or low friction coatings). To face problems arising from the multi-element nature and the often extremely narrow composition domain of CMAs, multisource coating methods as an alternative of deposition from alloy targets, and selected combinations of organometallic precursors will be studied. Dedicated reactors, appropriate operating conditions, state of the art diagnostics and characterization techniques will also be investigated.

MM 7 Hauptvortrag Peter Schall

Zeit: Freitag 14:00–14:30 Raum: TU H1058

Hauptvortrag MM 7.1 Fr 14:00 TU H1058

Colloidal Particles - a 3-D Analogue Computer for Materials Research — •Peter Schall[1], David A. Weitz[1,2], and Frans Spaepen[1] — [1]Division of Engineering and Applied Sciences, Harvard University, Cambridge MA, U.S.A. — [2]Department of Physics, Harvard University, Cambridge MA, U.S.A.

Colloidal suspensions are widely used to study a variety of phenomena in hard condensed matter physics. The particles - several ten nanometers to micrometers in size - self organize into structures similar to atoms in different phases of condensed matter. Crystalline as well as amorphous states can be prepared. Being several orders of magnitude larger than atoms, colloidal particles offer the unique possibility for studies at convenient length and time scales. The positions of the individual particles can be determined accurately in three dimensions using confocal microscopy. We perform deformation experiments on colloidal crystals and glasses to get deeper insight into atomic processes of plastic deformation. We show

that colloidal crystals exhibit dislocations in close analogy to dislocations in hard materials. Due to the larger size and the extended time scale of the colloidal particles, we are able to follow the nucleation of dislocations and their propagation in situ and on the particle scale. We also track the motion of the particles in amorphous suspensions and we are able to identify local shear events that give rise to the macroscopic deformation. We will present a variety of experiments on colloidal crystals and glasses, such as the epitaxial crystal growth on a stretched substrate, shear experiments, and "nano"indentation experiments using a conventional sewing needle as an indenter.

MM 8 Symposium Complex Metallic Alloys, Hauptvortrag Esther Belin-Ferré

Zeit: Freitag 14:45–15:15 Raum: TU H1058

Hauptvortrag MM 8.1 Fr 14:45 TU H1058

Electronic structure of Frank-Kasper Al-Mg based compounds — •Esther Belin-Ferré — Laboratoire de Chimie Physique Matière et Rayonnement, UMR 7614, 11 rue Pierre et Marie Curie, 75231 Paris cedex 05, France

In the Al-Mg Frank-Kasper system, the stable crystalline β-Al_3Mg_2 compound possesses a large cubic unit cell decorated with a complex packing of tetrahedral and icosahedral clusters. Furthermore, quasiperiodic compounds are found in the Al-Mg as well as Al-Mg-Zn systems. The electronic structure of these complex intermetallic compounds was investigated using X-ray emission and X-ray photoabsorption spectroscopy techniques, which allow us to describe separately the energy distribution of occupied and unoccupied states around Al and (or) Mg elements in the solid. The data are averaged over the various Al and (or) Mg sites. The paper will report and discuss these spectroscopic data with emphasis put on the β-Al_3Mg_2 compound. In this compound, the Al and Mg electronic distributions depart from that in the pure Al and Mg metals. A faint pseudo-gap is found at the Fermi level, indicating that in spite of its complex atomic structure, β-Al_3Mg_2 still retains metallic character.

MM 9 Symposium Complex Metallic Alloys II

Zeit: Freitag 15:15–16:30 Raum: TU H1058

MM 9.1 Fr 15:15 TU H1058

Prinzipien der Strukturbildung in kondensierter komplexer Materie — •P. Häussler, J. Barzola-Quiquia, W. Rauchhaupt, M. Stiehler und D. Hauschild — TU Chemnitz, Institut für Physik, 09107 Chemnitz

In ungeordneten Systemen zeigt sich immer deutlicher, dass räumlich begrenzte, sphärisch-periodische Anordnungen der Atome um jedes Aufatom existieren (Spiegelsphären statt Spiegelebenen wie im Kristall). Diese sphärisch-periodische Ordnung (SPO) bildet sich durch eine sich selbst organisierende Optimierung einer Resonanz zwischen den Valenzelektronen als Ganzem und der sich bildenden statischen Struktur. SPO ist somit das Ergebnis eines globalen Ordnungsmechanismus, der die lokale Quantenchemie ergänzt. Es wurde dabei registriert, dass SPO sowohl bei flüssigen und amorphen metallischen Systemen, aber auch Halbleitern, Isolatoren, Quasikristallen, 1/2Heusler-Legierungen und ionisch gebundenen Systemen auftritt. Verschiedentlich treten Winkelkorrelationen als weiteres resonanz-induziertes Ordnungsphänomen auf. Ob ein System elektrisch leitend ist, hängt von der Stärke der Resonanzen ab, da sich, korreliert mit diesen, eine Energielücke an der Fermikante bildet (Peierlsartig).

Es werden im Vortrag die bis heute bekannten verschiedenen Szenarien der Optimierung der Resonanzen vorgestellt. Da flüssige und amorphe Systeme die Prekursoren für Kristalle sind, sind die beschriebenen Mechanismen von grundsätzlicher Bedeutung.

MM 9.2 Fr 15:30 TU H1058

The atomic pair distribution function (PDF) as a nano-scale structure probe for CMA — •Stefan Brühne[1], Eckhard Uhrig[1], Michael Feuerbacher[2], and Wolf Assmus[1] — [1]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Robert-Mayer-Str. 2-4, D-60054 Frankfurt am Main — [2]Institut für Mikrostrukturforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich

The local atomic structure of any condensed matter is accessible via the atomic pair distribution function (PDF) from powder diffraction. We recently succeeded in unraveling the local structure of some icosahedral Mg-Zn-*RE* (*RE* = Y and Ho) alloys from in-house X-ray experiments in a sphere of 5.4 nm. Synchrotron data yield better resolved PDFs though they result in the same structural units of ∼1.5 nm in diameter. The method also applies well to the investigation of inherent disorder of Complex Metallic Alloys (CMA). The local structures of the Mg-Zn binaries $MgZn_2$ (hP12) and Mg_4Zn_7 (mC110) are discussed: The different length scales of the local structures *vs.* large translations become directly visible. The PDF of β-Al_3Mg_2 (cF1832-664, $a \approx 2.8$ nm), one of the most complex CMA in terms of unit cell dimension and atomic disorder, is examined. PDF will serve as a probe for monitoring the local atomic structure in the course of tailoring CMA structures w.r.t. their physical and mechanical properties.

MM 9.3 Fr 15:45 TU H1058

Investigation of Ti-Base Alloys with Positron Annihilation Techniques — •Falko Baier[1], Wolfgang Sprengel[2], and Mariana Calin[3] — [1]Physical Metallurgy, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt — [2]ITAP, Stuttgart University, Pfaffenwaldring 57, 70550 Stuttgart — [3]Materials Science and Engineering, University Bucharest, Romania

The research and development of Ti-based alloys for biomedical applications is focused on the development of low rigidity beta-phase Ti alloys composed of non-toxic elements with good mechanical properties and workability. A major drawback of these alloys is their poor workability. In order to overcome these limitations lots of work has been spent in order to find new Ti-alloys by varying the compositions or modifying the existing ones for the improvement of the formability. We present measurements of the positron lifetime and coincident Doppler broadening of the positron-electron annihilation photon line in as-cast and deformed Ti-base alloys in order to show the advantages of this non-destructive method for the field of engineering applications, because the sensitivity of positrons to defects in plastically deformed metals has been well-known since the 1960s. The addition of the element-sensitive Doppler broadening technique gives access to the chemical nature of the dislocation environment.

MM 9.4 Fr 16:00 TU H1058

Structures and Properties of the Refractory Silicides Ti_5Si_3 and $TiSi_2$ — •Georg Frommeyer and Rainer Rosenkranz — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The refractory titanium silicides Ti_5Si_3 and $TiSi_2$ with complex hexagonal $D8_8$ and orthorhombic C54 lattice structures exhibit some superior physical and mechanical properties, such as high lattice energies and melting temperatures; high hardness, elastic stiffness and flow stresses; low densities and excellent creep and oxidation resistance. In addition titanium silicides possess appropriate electrical and thermal conductivity, and good compatibility to silicon and titanium substrates. Therefore, these silicides are also suitable for electronic interconnections, diffusion barriers and graded bioactive glass coatings The complex lattice structures and a large constribution of covalent bonding to the total binding energies of these compounds predestine these less common quasi intermetallics to be considered for high-temperature applications in the aviation and space industry.

MM 9.5 Fr 16:15 TU H1058

Surfaces of Al-rich complex metallic alloys — •Vincent Fournée[1], Amy Ross[2], Tom Lograsso[2], Jack Barrow[2], Masahiko Shimoda[3], An-Pang Tsai[3], and Patricia Thiel[2] — [1]LSG2M, CNRS-UMR7584, Ecole des Mines, Parc de Saurupt, 54042 Nancy, France — [2]Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA — [3]NIMS, 1-2-1 Sengen, Tsukuba-shi, Ibaraki 305-0047 Japan

Understanding the structure and physical behaviour of complex metallic alloy surfaces is of key importance. Up to now, most studies have been focused on the surface structure of Al-rich quasiperiodic alloys. It is found that the surface is formed at dense Al-rich layers of the bulk structure, with no reconstruction. This result is rather surprising as even for simpler systems like periodic bimetallic alloys, surface truncation of the bulk structure can give rise to atomic and chemical rearrangements, including surface relaxation, modification of the bulk periodicity (reconstruction) or the chemical composition (surface segregation). Here, we have investigated the surface structure of some related periodic alloy phases, namely the xsi-AlPdMn approximant, which is an orthorhombic crystal with a large unit cell. The surface perpendicular to its pseudo ten-fold axis was investigated by STM, LEED and XPD. The surface structure can also be interpreted as bulk-terminated, corresponding to dense Al-rich layers of the bulk structure. Similarities and differences between the quasicrystal and its periodic approximant will be outlined.

MM 10 Symposium Complex Metallic Alloys, Hauptvortrag Janez Dolinsek

Zeit: Freitag 17:00–17:30 Raum: TU H1058

Hauptvortrag MM 10.1 Fr 17:00 TU H1058

Magnetic and Transport Properties of Al-based Complex Metallic Alloys — •Janez Dolinsek — J. Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

Complex Metallic Alloys (CMA) are intermetallic compounds with crystal structures based on giant unit cells with an edge length of several nanometers and containing many tens up to more than a thousand atoms per unit cell. The examples are β-Al3Mg2 (1168 atoms/u.c.), orthorhombic ξ'-Al74Pd22Mn4 (320 atoms/u.c.) with its Ψ-modification (about 1500 atoms/u.c), etc. Recently, high-quality samples of orthorhombic Al-Cr-Fe, ξ'-Al-Pd-Mn and Ψ-Al-Pd-Mn giant-unit-cell materials were prepared and their physical properties were studied. The electrical resistivities show very weak (or no) temperature dependence between room temperature and 4 K. The magnetic susceptibility shows the existence of a tiny fraction (of about 1 percent for the Al-Cr-Fe samples and about 100 ppm for the ξ'-Al-Pd-Mn and Ψ-Al-Pd-Mn) of localized magnetic moments with Curie-like temperature dependence. Thermal conductivity measurements show that the electronic and lattice contributions are of comparable size. The thermoelectric power can be either positive or negative with a complicated temperature dependence.

MM 11 Symposium Complex Metallic Alloys III

Zeit: Freitag 17:30–18:45 Raum: TU H1058

MM 11.1 Fr 17:30 TU H1058

Crack propagation in complex metallic alloys — •Frohmut Rösch[1], Peter Gumbsch[2,3], and Hans-Rainer Trebin[1] — [1]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart — [2]Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen, 76131 Karlsruhe — [3]Fraunhofer Institut für Werkstoffmechanik, 79108 Freiburg

Intermetallic compounds frequently combine interesting properties like high melting point, high-temperature strength, and low density. However, possible applications are then often limited by extreme brittleness at low or ambient temperatures. To develop new materials it is essential to understand crack behaviour on an atomistic level. As experiments on this length scale are difficult, computer simulations are the method of choice to reveal the fundamentals of fracture.

We investigate crack propagation by molecular dynamics simulations with model potentials in an icosahedral model quasicrystal and in a C15 Laves phase. In the quasicrystal the roughness of the fracture surfaces is determined by clusters, whereas in the Laves phase the cleavage planes are rough only on an atomic scale. In both materials the crack path cannot be determined by a simple energy criterion. As a step towards realistic simulations of complex metallic alloys, we also present first results with Embedded Atom Method potentials for C15-$NbCr_2$.

MM 11.2 Fr 17:45 TU H1058

The phasonic degree of freedom in the Ξ-Al-Pd-Mn phases: Metadislocations and phasonic phase boundaries — •Michael Engel und Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

One of the properties which distinguishes complex metallic alloys from ordinary metallic alloys is the possibility of spatial rearrangements of the cluster substructure resulting in new unit cells. Such rearrangements are discrete degrees of freedom, well known for another class of complex metallic compounds, quasicrystals, which can be seen as CMAs with infinite unit cells. By adopting quasicrystal terminology, the degrees of freedom are called phasonic degrees of freedom.

We demonstrate that the Ξ-(AlPdMn)-phases ξ, ξ', and ξ'_n can be modelled by a simple projection formalism in three-dimensional hyperspace. It follows that in the ξ'_n-phases there is one phasonic degree of freedom, whose excitation results in a movement of structural defects, so-called phason-planes. Furthermore we describe phasonic phase boundaries between different Ξ-phases and metadislocations, which are special textures of partial dislocations. Both are modelled geometrically in the hyperspace and compared to HREM images from the literature. We determine the metadislocations of lowest energy and relate them uniquely to experimentally observed ones. Since moving metadislocations in the ξ'-phase create new phason-planes, we suggest a dislocation induced phase transition from ξ' to ξ'_n.

MM 11.3 Fr 18:00 TU H1058

Plastic behaviour of polycrystalline β-Al-Mg — •Michael Feuerbacher and Marc Heggen — Institut für Festkörperforschung Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

$\beta - Al_3Mg_2$ is a cubic complex metallic alloy phase with particularly large lattice constants of 28.2 Å and 1168 atoms per unit cell. The main structural elements are Friauf polyhedra arranged in fivefold coordinations. The material is potentially interesting for technological applications since it is a lightweight alloy (2.2 g/cm^3) and it congruently solidifies from the melt.
We have performed uniaxial plastic deformation experiments on polycrystalline β-Al-Mg in the temperature range from 300 to 400 °C at strain rates of 10^{-4} and 10^{-5} s^{-1}. The material is highly ductile and shows strong continuous work softening after the upper yield point. We have performed stress-relaxation and temperature-cycling tests to determine the thermodynamic activation parameters of the deformation process. Strongly stress dependent activation volumes in the range of 0.3 to 2.2 nm^3 and a stress exponent of about 3.5 were found. The activation enthalpy assumes rather high values of 3 to 5 eV. After deformation the samples show strong shear bands oriented at 45 ° with respect to the compression axis.

MM 11.4 Fr 18:15 TU H1058

Structural defects in orthorhombic $Al_{13}Co_4$ — •Dewei Deng, Marc Heggen, and Michael Feuerbacher — Institut für Festkörperforschung Forschungszentrum Jülich GmbH

Orthorhombic $Al_{13}Co_4$ is a complex metallic alloy phase with 101 atoms per unit cell. The lattice constants are a= 0.8165(1)nm, b= 1.2352(1)nm, c= 1.4451(1)nm and it has a of $Pmn2_1$ space group. It is structurally isomorphic to the well investigated phase ξ'-Al-Pd-Mn in the sense that the [1 0 0] lattice direction of orthorhombic $Al_{13}Co_4$ can be described using similar types of hexagon-tiling arrangements as

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 $Al_{88}Y_7Fe_5$ — •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.

MM 14 Wachstum

Zeit: Freitag 14:45–16:15 Raum: TU H2038

MM 14.1 Fr 14:45 TU H2038

Auf der Suche nach einem Modellsystem zum Verständnis der Korrelationseffekte beim normalen Kornwachstum — •Anne-Catherine PROBST[1], Dmitri MOLODOV[2], Rainer BIRRINGER[1] und Carl E. KRILL[3] — [1]FR 7.3 Technische Physik, Universität des Saarlandes, Postfach 151150, 66041 SAARBRÜCKEN — [2]Institut für Metallkunde und Metallphysik, R.W.T.H. Aachen, Kopernikusstr. 14, 52056 AACHEN — [3]Abt. Werkstoffe der Elektrotechnik, Universität Ulm, Albert-Einstein-Allee 47, 89081 ULM

Die physikalischen Eigenschaften polykristalliner Materialien hängen in hohem Maße von der Größe der Kristallite ab. Dementsprechend ändern sich diese Eigenschaften, wenn Kornwachstum durch Anlassen bei hinreichend hohen Temperaturen induziert wird. Bisher gibt es keine Theorie, die das Kornwachstum einphasiger Materialien – sog. normales Kornwachstum – vollständig beschreibt. Insbesondere können analytische Modelle wie die mean-field-Theorie von Hillert die lognormale Form experimentell gefundener Korngrößenverteilungen überhaupt nicht erklären. Um dieses Defizit zu beheben, formulierte Wu eine neue, auf einem nicht-mean-field-Ansatz beruhende Wachstumstheorie, die explizit die Existenz einer Korngrößenkorrelation zwischen benachbarten Körner berücksichtigt. Es wurde ein Modellsystem für normales Kornwachstum gesucht, welches zur experimentellen Überprüfung des Wuschen Ansatzes dienen sollte.

MM 14.2 Fr 15:00 TU H2038

The size distribution induced by normal grain growth is lognormal in shape—fact or fiction? — •Carl E. Krill III[1], Max Ziehmer[2], and Lukas Helfen[3] — [1]Materials Division, Albert-Einstein-Allee 47, University of Ulm, D-89081 Ulm — [2]FR 7.3 Technical Physics, Geb. 43B, University of the Saarland, D-66123 Saarbrücken — [3]ESRF, BP 220, F-38043 Grenoble Cedex

Experimental investigations of normal grain growth invariably find that the distribution of grain sizes can be approximated by a lognormal function. Computer simulations of the same process, however, predict a far more symmetrical distribution shape, regardless of the underlying algorithm used to model the migration of grain boundaries. One possible explanation for this discrepancy arises from the manner in which the grain size is determined: in experiment, one generally relies on the cross-sectional area evident in a two-dimensional section passing through the grain, whereas one has access to the full three-dimensional grain volume during a simulation. By applying 2-D and 3-D grain-size analyses to identical polycrystalline microstructures, we have attempted to assess the extent to which stereological factors contribute to the apparent shape of the size distribution generated by normal grain growth. Results obtained using experimental coarsening data are compared to those of a large-scale grain-growth simulation, with the goal of determining whether the size distribution really differs in the two cases.

MM 14.3 Fr 15:15 TU H2038

Dendritic structure and solidification kinetics of undercooled Ni-Zr alloys — •Peter Galenko, Dieter Herlach, Gandham Phanikumar, and Oliver Funke — Intitut fuer Raumsimulation, DLR, 51170 Koeln, Deutschland

Ni-Zr droplets have been melted and undercooled in electromagnetic levitation facility. After controlled triggering of solidification, measurements of solidification velocity have been provided by capacity sensor technique and high-speed camera technique. Novel experimental results on the kinetics of solidification of undercooled Ni-Zr alloys are found. The velocity-undercooling relationship have been plotted for three contents of diluted Ni-Zr alloys and metallographic investigations of a crystalline structure have been performed. The microstructure of all samples is found to be a dendritic like. The microstructural features as a function of undercooling are attributed to morphological transitions, viz., from grain refined (GR) equiaxed microstructure to a coarse grained (CG) dendritic microstructure and to a grain refined (GR) equiaxed microstructure. The kinetics of dendritic growth in undercooled droplets are analysed using the local nonequilibrium solidification model [1]. The experimental values of critical undercoolings for the GR-CG-GR transitions are compared with the modeling predictions. The disagreement of the theoretical predictions are attributed to the influence of convective flow, especially, at small and moderate undercoolings.

The work was supported by DFG under contract No. He 1601/13.

[1] P.K. Galenko and D.A. Danilov, Phys. Lett. A 235 (1997) 271; J. Cryst. Growth 197 (1999) 992.

MM 14.4 Fr 15:30 TU H2038

Growth kinetics of dendrites in Ni and Ni–Zr systems: Simulations and experiments — •Denis Danilov[1], Peter Galenko[2], and Britta Nestler[1] — [1]Karlsruhe University of Applied Science, Karlsruhe, Germany — [2]German Aerospace Center, Cologne, Germany

The morphologies and the kinetics of dendritic microstructures in pure Ni as well as in Ni–Zr alloys are modeled using the phase-field simulations. The simulation results are compared with experimental data on solidified samples processed by electromagnetic levitation facility and with the solutions of a sharp-interface model. In particular, we consider the velocity–undercooling relations for different thermophysical data and for different compositions in 2D and 3D. We use a phase-field model for non-isothermal solidification in multicomponent systems consistent with the formalism of classic irreversible thermodynamics to perform the numerical simulations of the dendritic growth structures. 3D morphology transitions are obtained for variations in surface energy and kinetic anisotropies at different undercoolings. In computations, we investigate the convergence behaviour of a standard phase-field model and of its thin interface extension at different undercoolings and at different ratios between the diffuse interface thickness and the atomistic capillary length. The influence of the grid anisotropy is accurately analyzed for a finite difference method and for an adaptive finite element method in comparison. The work was supported by DFG under contracts No. Ne 882/2 and He 1601/13.

MM 14.5 Fr 15:45 TU H2038

Controlling of symmetry and fractal dimension of Xe dendrites by heating — •Marco Fell, Herman M. Singer und Jörg H. Bilgram — Laboratorium für Festkörperphysik, ETH, CH-8093 Zürich, Switzerland

Xenon dendrites, grown in supercooled melt ($\Delta T \sim 100 - 200$ mK), show characteristic sidebranching frequencies depending on supercooling. They are statistically symmetric and the contours' outlines have a characterictic fractal dimension, depending on morphologies: dendrite, seaweed and dendritic doublon.

We experimentally perform periodical heating of the melt close to the melting point and observe a change in the growth morphology of the crystal: The whole dendrite stops growing or even begins to melt, depending on power and duration of heating. After stopping the heating, the liquid xenon cools down and growth restarts. Interestingly four absolutely symmetrical lobes start to grow at the main tip.

This process is found to form crystals with a lower fractal dimension as well as a lower curvature of the contour than known in the morphologies for free growth.

MM 14.6 Fr 16:00 TU H2038

Interacting Xenon Dendrites — •Oliver Wittwer und Jörg Bilgram — Laboratorium für Festkörperphysik, ETH, CH 8093 Zürich, Switzerland

In our experiments we investigate in situ three dimensional pattern formation of xenon crystals during free growth. Well known morphologies are dendrites, doublons and seaweed. We also observe triplons and quadruplons. The transition from dendrite to doublon has gained interest since it has been discovered in metallic samples [1]. Transitions between these morphologies can be initiated in our experiments by changing the temperature distribution in the environment of a growing crystal [2].

In this communication we report on periodic oscillations in growth velocity induced by the interaction of two dendrites growing close to each other. The amplitude of these oscillations is in the range of 20% of tip velocity and increasing with time. These oscillations have to be compared with the growth velocity of a freely growing isolated dendrite where fluctuations in growth rate (mainly due to pixel noise) are below ±1.5% of tip velocity at the same experimental conditions.

[1] K. Dragnevski, R. F. Cochrane, and A. M. Mullis, Phys. Rev. Lett. **89**, 215502 (2002)

[2] I. Stalder and J. H. Bilgram, Europhys. Lett. **56**, 829 (2001)

MM 15 Hauptvortrag Yves Bréchet

Zeit: Samstag 08:30–09:00 Raum: TU H1058

Hauptvortrag MM 15.1 Sa 08:30 TU H1058

Modelling of phase transformations : from the lab to the plant — •Yves J.M. Bréchet — L.T.P.C.M., Domaine Universitaire de Grenoble, BP75 , F-38402 Saint Martin d'Hères

Traditionnally, the interest of physicists for phase transformations in the metallic solid state has been focussed either on order-disorder transitions, or on phase separation involving nucleation and growth or spinodal decomposition. In these problems, the techniques from statistical physics (Monte Carlo simulation) as well as the continuum approaches have proven to be very powerfull. However, "real life"as encountered in industrial situations , require complementary approaches: dealing with long time behaviour and the role of vacancies on the selection of kinetic path, dealing with non isothermal heat treatments such as the ones obtained during welding, dealing with other types of transformations involving interface migration and allotropic transformations. In turn, these questions driven by the side of application generate very fundamental questions on the coupling between thermodynamics and kinetics which might renew the interest of the physics community for these problems. The present contribution will illustrate on some examples from the physical metallurgy of steel and aluminium alloys the values and limits of the current approaches.

MM 16 Phasenumwandlung I

Zeit: Samstag 09:15–10:45 Raum: TU H1058

MM 16.1 Sa 09:15 TU H1058

In-situ observation of Short Range Order and Precipitation Processes in Ti-V by High Energy X-Ray Diffraction — •Ingo Ramsteiner, Andreas Schöps, Harald Reichert, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Stuttgart

Phase transformations, especially precipitation processes, are a key factor in alloy design. Therefore, they are of major interest in materials science. Understanding these processes in the framework of statistical thermodynamics requires knowledge about the atomic interaction potentials between the alloy constituents. Experimentally, these parameters can be accessed via the diffuse scattering caused by the configurational short range order (SRO) and lattice distortions. With the high energy monochromatic Laue technique we present a tool to study both phenomena simultaneously in situ in the bulk of a macroscopic single crystal. Recording the scattered intensity with a 2D detector reveals distinct precipitate Bragg peaks embedded into the diffuse scattering of the matrix.

We present an in situ case study of bcc Ti-V. Apart from the SRO, growth and dissolution of two different types of precipitates are observed, depending on the anneal temperature. HRTEM experiments have been conducted to complement and verify our results.

MM 16.2 Sa 09:30 TU H1058

Die oberflächennahe Mikrostruktur von Pt-Rh — •Ch. Steiner[1], M.M.I.P. van der Klis[1], B. Schönfeld[1], G. Kostorz[1], B. Patterson[2] und P. Willmott[2] — [1]ETH Zürich, Institut für Angewandte Physik, CH-8093 Zürich, Schweiz — [2]Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI, Schweiz

Mit Synchrotronstrahlung unter streifendem Einfall wurde die diffuse Streuung an einer (110)-Oberfläche von Pt-47 at.% Rh gemessen. Die Probe befand sich in einer UHV-Umgebung bei 1000 K. Nach Abtrennung von thermisch diffuser Streuung und Compton-Streuung wurde der elastische Anteil in Nahordnungsstreuung und lineare Verzerrungsstreuung separiert. Wie bei einer früher durchgeführten Volumenmessung an Pt-47 at.% Rh zeigt die Nahordnungsstreuung auch nahe der Oberfläche ein Vorliegen lokaler Ordnung an. Die Asymmetrie in der Verzerrungsstreuung, zuvor deutlich in der Nähe der Bragg-Reflexe zu erkennen, ist jetzt weniger stark ausgeprägt. Im Unterschied zu Untersuchungen in der Literatur, die bei Zimmertemperatur an einer Pt-50 at.% Rh(110)-Oberfläche durchgeführt worden waren, wurde keine Rekonstruktion gefunden.

MM 16.3 Sa 09:45 TU H1058

Leerstellenpfad und Ordnungskinetik — •David Reith[1], Wolfgang Püschl[1], Wolfgang Pfeiler[1] und Ferdinand Haider[2] — [1]Inst. f. Materialphysik, Universität Wien — [2]Inst. f. Physik, Universität Augsburg

Mit einem Wartezeit-Monte-Carlo Algorithmus wurde die Bewegung von Leerstellen in Intermetallischen Verbindungen vom Typ $L1_2$ und B2 im geordneten und ungeordneten Zustand untersucht. Die Zeit, die benötigt wird, um einen vorgegebenen Anteil (z.B. 90%) der Gitterplätze in der Rechenzelle mindestens einmal zu besuchen, ergibt sich als proportional zur Größe der Rechenzelle und damit indirekt proportional zur Leerstellendichte. Die fast vollständige Überdeckung der Rechenzelle mit Leerstellenbesuchen stellt die Voraussetzung dafür dar, dass ein Phasenübergang homogen und nicht nur in einzelnen Wanderungsbereichen der Leerstelle abläuft. Aus den rechnerisch ermittelten Proportionalitätsfaktoren kann eine Beziehung für den Zeitpunkt des Überganges von heterogenem zu homogenem Verhalten in Abhängigkeit von Leerstellenkonzentration und Wanderungsenthalpie aufgestellt und graphisch dargestellt werden. Dieses ist besser begründet als ein früher von uns verwendeter Ansatz, bei dem die mittleren quadratischen Wanderungsdistanzen herangezogen wurden (Intermetallics 11 (2003) 161).

MM 16.4 Sa 10:00 TU H1058

Influence of Twin Grain Boundaries on Texture Evolution during α-γ-Phase Transformation in Microalloyed Steels — •Ingo Lischewski und Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, D-52056 Aachen, Germany

The partial ferrite to austenite phase transformation in microalloyed steel was studied, with a special focus on the influence of twinning on the texture evolution. During the diffusion controlled phase transformation a texture memory effect takes place. This effect is explained by different orientation relationship models. The present models are not capable of quantitatively predicting the texture changes during phase transformation. Various mechanisms known that cause a texture change. This study demonstrates the influence of twin formation on the transformation texture.

Samples of a microalloyed steel were wrapped in a CrNi-18/9 steel foil and annealed at a low transformation temperature. Nickel is believed to diffuse from the steel wrapping into the sample, and to stabilize the austenite and retain it on cooling to ambient temperature. This allows us to measure locally by EBSD the orientation of the ferrite prior to transformation and at the same location the orientation of the austenite subsequent to transformation. The measurements were conducted in a high resolution FEG-SEM.

The study demonstrates an influence of twin grain boundaries on the development of transformation textures. Mainly $\Sigma 3$ und $\Sigma 9$ twin grain boundaries in the austenite phase are observed. The twin grain boundaries are not randomly distributed over the whole microstructure.

MM 16.5 Sa 10:15 TU H1058

Ab initio based free energy surfaces: A powerful tool to derive temperature dependent thermodynamic and kinetic parameters — •Blazej Grabowski — Uni Paderborn

Blazej Grabowski, Sixten Boeck, Jörg Neugebauer Uni Paderborn MPI für Eisenforschung Düsseldorf

Many metals and alloys exhibit a complex pressure and temperature dependent phase diagram. The common approaches to theoretically predict these diagrams are based on empirical interpolation schemes in connection with experimental input data. The ab initio calculation of free energy surfaces as function of relevant reaction coordinates (e.g. lattice constant, c/a ratio) provides a direct tool to identify stable and metastable equilibrium configurations, reaction barriers and reaction pathes by fully including temperature effects. In order to test the applicability and accuaracy of this approach we have implemented an efficient scheme in our plane wave pseudopotential code (SFHIngX) to calculate free energy surfaces employing the quasi harmonic approximation. The method has been applied to map the free energy surface of several metals (Al, Fe). The results are compared with experiment.

MM 16.6 Sa 10:30 TU H1058

Interface thermodynamics of multi-layered systems — •Ferdinand Sommer — MPI for Metals Research, Stuttgart

The basic objective is to understand the formation and stability of the interface(s) and the interface phases (amorphous or crystalline) that are developed between thin metallic layers in contact. The driving force for the formation of interface phases of multilayered systems has been evaluated. Surface and interface energies and the enthalpy of formation of interface phases have been analysed on the basis of the Miedema model[(1)]. The entropy contributions are derived from a model developed for the excess entropy of solutions[(2)]. Some results are compared with experimental data.

(1) F. R. de Boer, R. Boom, W. C. M. Mattens and A. K. Niessen, in Cohesion in Metals: Transition Metal Alloys, North Holland, Amsterdam (1988)

(2) F. Sommer, R.N. Singh and V. Witusiewicz, J. Alloys Comp. 325 (2001) 118

MM 17 Phasenumwandlung II

Zeit: Samstag 11:00–12:15 Raum: TU H1058

MM 17.1 Sa 11:00 TU H1058

Ausscheidungen in Al-Cu und Al-Ag: Strukturbestimmung mit ab-initio Rechnungen — •Michael Röbel und Torsten E.M. Staab — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friederich-Wilhelms Universität Bonn, Nußallee 14-16, D-53115 Bonn, Germany

Aluminium ist als moderner Werkstoff aus dem Leichtbau nicht mehr wegzudenken. Seine Werkstoffeigenschaften werden maßgeblich durch Ausscheidungen von Legierungselementen beeinflusst. Um einen tieferen Einblick in den strukturellen Aufbau der einzelnen ausgeschiedenen Phasen zu gewinnen, wurden ab-initio Rechnungen mit SIESTA durchgeführt. Die Berechnungen wurden gemäß der Ausscheidungssequenz von Al-Cu Legierungen an Guinier-Preston Zonen I und II, der Θ'-Phase und der stabilen Θ-Phase des überalterten Werkstoffes vorgenommen. Im Vergleich zu Al-Ag zeigt sich der Einfluss der Gitterkonstanten des Legierungselementes relativ zu der des Wirtsgitters auf den Formfaktor der Ausscheidung. Mit den relaxierten Atomkoordinaten lassen sich experimentelle Parameter wie die Positronenlebensdauer berechnen. Dies ermöglicht eine bessere Interpretation von Messungen.

MM 17.2 Sa 11:15 TU H1058

Untersuchungen zur inneren Oxidation in Ni-Zr-Y-Legierungen — •Bärbel Kloss, Uwe Glatzel und Rainer Völkl — Universität Bayreuth, Lehrstuhl Metallische Werkstoffe, Ludwig-Thoma-Str. 36b, 95440 Bayreuth

Nickellegierungen mit geringen Zusätzen an Zr und Y wurden bei 1000°C unter geringem Sauerstoffpartialdruck wärmebehandelt. Unter den gegebenen Versuchsbedingungen fand eine innere Oxidation statt. Von besonderem Interesse waren die Morphologie und Struktur der gebildeten Oxidteilchen sowie die Kinetik der Oxidationsprozesse, die experimentell bestimmt und mit theoretisch ermittelten Werten verglichen wurde. Die Oxidationsgeschwindigkeit von binären Ni-Zr-Legierungen stimmt mit der Theorie überein. Ternäre Ni-Zr-Y-Legierungen zeigen hingegen einen um mehrere Größenordnungen schnelleren Oxidationsverlauf als theoretisch vorausgesagt. Bereits geringe Zusätze an Y wirken beschleunigend auf die Oxidationskinetik. Dieses Phänomen ist nicht mehr mit der allgemeinen Theorie zur inneren Oxidation zu erklären, sondern beruht auf der Verbesserung der Sauerstoffleitfähigkeit des gebildeten Zirkonoxids durch die Zugabe von Y. Weitere Untersuchungen erfolgten bei höheren Wärmebehandlungstemperaturen (1100°C, 1200°C). Dabei wird bei 1200°C ein anderer Oxidationsmechanismus als bei 1000°C beobachtet.

MM 17.3 Sa 11:30 TU H1058

Determination of Atomic Interaction Parameters from X-Ray Diffuse Scattering in the Binary Alloy System Ni-Pd — •Markus Mezger[1,2], Harald Reichert[1], and Helmut Dosch[1,2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart — [2]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, Pfaffenwaldring 57, D-70550 Stuttgart

Macroscopic properties of alloys, such as the elastic constants, are determined by the atomic interaction potential between the different alloy components. These parameters are encoded in the diffuse scattering caused by configurational short range order (SRO) and lattice distortions in the disordered phase. For the Ni-Pd alloy system we present a method to obtain the interaction parameters directly from X-ray diffuse scattering. In order to collect the experimental data in-situ meassurements on macroscopic $Ni_{55}Pd_{45}$ and $Ni_{25}Pd_{75}$ single crystals were performed in the temperature range from 20 °C up to 900 °C. For the data analysis a formalism based on the spherical model and the Kanzaki-force concept has been used within a simulated annealing algorithm.

MM 17.4 Sa 11:45 TU H1058

Solitons and the ω-phase in Bcc Crystals — •Johannes Roth — Institut für Theoretische und Angewandte Physik, Universität Stuttgart

Molecular dynamics simulations have been applied to generate shock waves in bcc crystals. The interaction between the atoms has been modelled by the Dzugutov potential[1]. If the shock front is slower than the speed of sound a transition to the hexagonal ω-phase[2] is observed with a kink as phase boundary. If the shock front velocity becomes faster than the speed of sound the ω-phase is replaced by solitons, and we can show that both phenomena are closely related. The origin of the ω-phase and its stability will be discussed. The interaction of the solitons has been studied and the collision property has been demonstrated. For the original Dzugutov potential the solitons decay through transversal fluctuations. We describe how the potential has to be modified to suppress this instability.

[1] M. Dzugutov, J. Non-Cryst. Sol. **131** (1991) 62
[2] S.K. Sikka, Y.K. Vohra, R. Chidambaram, Prog. Mat. Sci. **27** (1982) 245

MM 17.5 Sa 12:00 TU H1058

Structural Phase Transition in Tb5(Si0.6Ge0.4)4 at Low Temperature — •Andreas Kupsch[1,2], Alexandr Levin[1], Dirk C. Meyer[1], and Peter Paufler[1] — [1]Institut für Strukturphysik, TU Dresden, 01062 Dresden — [2]BAM, VIII.32, 12200 Berlin

The occurrence of the giant magnetocaloric effect (MCE) has been measured with various rare earth- Si/Ge compounds. The magnetic phase transition from the high temperature paramagnetic to the low temperature ferromagnetic phase is accompanied by a structural phase transition. We report on crystallographic details of a transition measured with powdered Tb5(Si0.6Ge0.4)4 at low temperatures (150 and 130 K), for which the MCE was observed at Tc = 150 K . The pseudo-binary compound is monoclinic at room temperature (P1121/a). Changes of reflection intensities and positions in the diffraction patterns indicate a structural phase transition between 150 K and 100 K, where the compound orders in an orthorhombic structure (Pnma). Split-up crystallographic sites of the monoclinic unit cell degenerate to sites of higher symmetry in the orthorhombic structure. It turned out that both phases coexist at the selected temperatures but the phase content changes significantly. As already reported for Gd5Si2Ge2 the key feature of the structural phase transition is a shear movement of pairs of flat atomic units along the crystallographic a direction by 0.84 Å and tremendous changes of selected (Si/Ge)-(Si/Ge) distances up to 0.95 Å.

MM 18 Nanoskalige Materialien I

Zeit: Samstag 09:15–10:45 Raum: TU H111

MM 18.1 Sa 09:15 TU H111

Untersuchungen an sauerstoffdotiertem nano-Ni — •Z.Q. Guan, X.M. Li, H. Wolf und Th. Wichert — Technische Physik, Universität des Saarlandes, D-66123 Saarbrücken

Das Kornwachstum in nanokristallinem Ni (nano-Ni) lässt sich durch Sauerstoffdotierung unterdrücken. Dadurch wird die thermische Stabilität des nanokristallinen Materials verbessert. Mit der Methode der gestörten $\gamma\gamma$-Winkekorrelation (PAC) wurden Untersuchungen durchgeführt, die zum mikroskopischen Verständnis der Mechanismen beitragen, die zur Stabilisierung von nano-Ni durch Sauerstoffdotierung führen. Die sauerstoffdotierten nano-Ni Proben wurden mit der Methode der gepulsten Elektrolyse hergestellt. Der Sauerstoffgehalt wurde durch Variation der Präparationsbedingungen kontrolliert und für drei unterschiedlich präparierte Proben durch Heißextraktion und EDX bestimmt; außerdem wurde auf der Basis der PAC Daten eine entsprechende Abschätzung vorgenommen. PAC Spektren, die direkt nach der Präparation aufgenommen wurden, legen nahe, dass Sauerstoff zum Teil in den Kristalliten gelöst ist. Gleichzeitig konnten keine Ausscheidungen von NiO detektiert werden. Nach sukzessivem Anlassen wurde festgestellt, dass im Bereich von 473 bis 773 K der Sauerstoffgehalt in den Ni Kristalliten zunimmt, oberhalb von 773 K aber wieder abnimmt. Diese Effekte werden hinsichtich der Zunahme auf Korngrenzenwanderung und hinsichtlich der Abnahme auf die Diffusion der Sauerstoffatome in die Korngrenzen zurückgeführt. Nach Tempern oberhalb von 1073 K wird die Bildung von NiO-Ausscheidungen beobachtet.

Gefördert durch die DFG im Rahmen des SFB 277.

MM 18.2 Sa 09:30 TU H111

MICROSTRUCTURAL EVOLUTION OF ULTRA-FINE GRAINED ECAP COPPER DURING ANNEALING — •Sheila Bhaumik, Myrjam Winning, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikussrt. 14, 52056 Aachen

The reduction of the grain size down to the submicrometer regime opened new and fascinating aspects for research in several fields of materials science. One of the most important characteristics of ultra-fine grained or nanocrystalline materials is that with decreasing grain size the ratio between surface and volume strongly increases, so that the properties of the internal interfaces become more and more important. On the other hand volume effects like dislocation multiplication are hindered or even suppressed. The structure as well as the thermal stability of massive ultra-fine grained copper was investigated. The used samples were produced by severe plastic deformation using the ECAP method (equal channel angular pressing). The influence of grain boundary triple junctions and the influence of the deformation character of the microstructure on the thermal behavior was investigated by ex-situ investigations using SEM/EBSD for increasing number of the ECAP passes. The experiments were designed to yield information on the correlation between the microstructure of ultra-fine grained materials and its stability against recrystallization and grain growth.

MM 18.3 Sa 09:45 TU H111

Direct Determination of Cation Disorder in Nanoscale Spinels by High-Resolution Magic-Angle Spinning Nuclear Magnetic Resonance Spectroscopy — •Vladimir Šepelák[1], Sylvio Indris[2], Klaus Dieter Becker[3], and Paul Heitjans[2] — [1]Center for Solid State Chemistry and New Materials, University of Hannover, 30167 Hannover, Germany; on leave from Slovak Academy of Sciences, Košice, Slovakia — [2]Institute of Physical Chemistry and Electrochemistry, University of Hannover, 30167 Hannover, Germany — [3]Institute of Physical and Theoretical Chemistry, Technical University of Braunschweig, 38106 Braunschweig, Germany

Complex oxides AB_2O_4 with the spinel structure, in general, and Al-containing members of this structural group, in particular, have continuously attracted interest because of the large diversity and the practical usefulness of their physical and chemical properties. Ultrafine powders of $MgAl_2O_4$ with crystallite sizes in the nm range have been prepared by high-energy milling the bulk material in a SPEX 8000 shaker mill using grinding chamber and balls made of ZrO_2. The nanoscale nature of the mechanically activated samples has been characterized by TEM, XRD and BET methods. The disorder of Mg^{2+} and Al^{3+} cations between the tetrahedral (A) and octahedral [B] sites in nanosized milled $MgAl_2O_4$ has been determined by ^{27}Al magic-angle spinning NMR spectroscopy. Disorder, measured by the fraction of Al^{3+} cations on (A) sites and described by the degree of inversion, λ, increases with increasing milling time. The cation inversion parameter of the nanoscale spinels is compared with that of the bulk materials quenched from high temperatures.

MM 18.4 Sa 10:00 TU H111

Charge-Induced Strain of Nanoporous Gold-Platinum Alloys — •Smrutiranjan Parida[1], Dominik Kramer[1], and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Universität des Saarlandes, Fachrichtung Technische Physik, Saarbrücken

If porous, nanostructured metals immersed in an electrolyte are charged electrically, volumetric expansion and contraction is induced in phase with the applied potential [1,2], with strain amplitudes comparable to those of commercial piezoceramics [1]. It has been shown that such nanoporous metal/electrolyte actuator materials can be prepared by dealloying [2], the selective dissolution of the less noble components of an alloy. We present in-situ measurements of the charge-induced strain of nanoporous gold-platinum alloys prepared by dealloying of silver-gold-copper-platinum alloys. The observed strain amplitudes increase with increasing platinum content for the composition studied. The maximum strain amplitudes are very large - larger by one order of magnitude compared to nanoporous gold prepared by dealloying Ag75Au25.

[1] J. Weissmüller et al, Science 300 (2003) 312 [2] D. Kramer, R. N. Viswanath, J. Weissmüller, Nano Letters 4 (2004) 793

MM 18.5 Sa 10:15 TU H111

Aktive Verformungsmechanismen in nanokristallinem Palladium als Funktion der Korngröße und der Dehnungsrate — •Jürgen Markmann[1,2], Harald Rösner[1] und Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut fur Nanotechnologie, Postfach 3640, 76021 Karlsruhe — [2]Universität des Saarlandes, FR 7.3 Technische Physik, Postfach 151150, 66041 Saarbrücken

Da Versetzungsquellen vom Frank-Read Typ aufgrund ihrer unrealistisch hohen Aktivierungsspannungen in Körnern, die nur einige Nanometer groß sind, nicht aktiv sein können, müssen andere Verformungsmechanismen die Duktilität von nanokristallinen (nk) Metallen bereitstellen. Ermöglicht durch die geringe Korngröße, kommen außer versetzungsbasierten Mechanismen, bei denen die Korngrenzen als Versetzungsquellen wirken, auch Korngrenzengleiten und Kornrotation in Frage. In dieser Studie werden die experimentellen Daten von Walzverformungen edelgaskondensierter nk Palladiumtabletten mit Literaturdaten der Verformung anderer fcc Metallen aus Experimenten und Simulationen in Bezug gesetzt. Abhängig von der Korngröße des betrachteten Metalls und der Dehnungsrate, mit der die Verformung erfolgt, stellen sich verschiedene Verformungsmechanismen und dazugehörige Akkommodationsmechanismen ein. Auf dieser Grundlage konnte ein Entwurf einer Verformungsmechanismenkarte für nanokristalline fcc Metalle entwickelt werden.

MM 18.6 Sa 10:30 TU H111

Nanocharacterization of magnetoresistant oxide tunnel barrier structures — •Mario Kuduz[1], Guido Schmitz[2], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Institut für Materialphysik, Universität Münster

Oxide tunnel barriers (TMR = Tunnel Magneto Resistance) are currently of interest for application in magnetic sensor and storage devices. Compared to Giant Magneto Resistance (GMR) devices, tunnel barriers are distinguished by an improved effect amplitude and a higher base resistivity, so that they may be used in "current perpendicular to plane" arrangements.

In this work the nano-structure of TMR devices in as-prepared state also as after annealing at temperatures of 150°C up to 500°C using field ion microscopy in combination with a 2D-detection setup was investigated. Spin valve structures consisting of Co and Ni(79) Fe(21) electrodes separated by aluminum-oxide barriers were prepared by ion beam sputter deposition on tips of 30 to 50nm radius of curvature suitable for field ion microscopy (FIM). In spite of the isolating character of the barrier

material, the chemical structure can be reasonably characterized by analytical field ion microscopy. The 3D spatial distribution of the atomic species and the diffusion behavior is discussed in dependence on the annealing temperatures.

MM 19 Nanoskalige Materialien II

Zeit: Samstag 11:00–12:30 Raum: TU H111

MM 19.1 Sa 11:00 TU H111

Der Einfluß der Mikrostruktur auf die magnetischen Eigenschaften der WC/Co Hartmetalle — •Irena Topic, Hans Georg Sockel und Mathias Göken — Lehrstuhl für Allgemeine Werkstoffeigenschaften, Friedrich-Alexander Universität Erlangen-Nürnberg, Martensstraße 5, 91058 Erlangen

Wolframkarbid-Kobalt Hartmetalle (WC/Co) sind Verbundwerkstoffe, die aus Wolframkarbidteilchen und Kobalt durch Sintern hergestellt werden. Die Kombination der harten WC-Partikel mit einer duktilen Kobaltmatrix führt zu attraktiven Werkstoffeigenschaften, wie hoher Verschleißfestigkeit und Zähigkeit. Wegen ihrer hervorragenden mechanischen Eigenschaften werden diese Werkstoffe in der Regel in der Schneidwerkzeugindustrie eingesetzt.
Bei diesen Werkstoffen wird Magnetismus häufig als einfache Qualitätssicherungsmaßnahme eingesetzt, um ihre Mikrostruktur zu charakterisieren. Eine empirische Beziehung zwischen den magnetischen Kenngrößen und den mikrostrukturellen Parametern wurde für die konventionellen und ultrafeinkörnigen Hartmetalle bestimmt. Ein starker Einfluß der WC Korngröße auf die Koerzitivfeldstärke wurde nachgewiesen. Zugleich wurde festgestellt, dass die dünnen Kobaltbereiche, die Zusammensetzung und die magnetokristalline Anisotropie des Kobalts auch einen großen Einfluß auf das magnetische Feld haben.

MM 19.2 Sa 11:15 TU H111

Grain size effect on the temperature dependence of the electric field gradient — •X.M. Li, Z.Q. Guan, H. Wolf, and Th. Wichert — Technische Physik, Universität des Saarlandes, D-66123 Saarbrücken

In many non-cubic bulk metals the temperature dependence of the electric field gradient (EFG) can be described by a $T^{3/2}$ dependence. Some theoretical models considering the electronic structure and the influence of phonons have been presented in the literature in order to explain this relation. Since it is expected that a reduction of the grain size to nanometer scale affects the electronic structure as well as the phonon spectrum, the temperature dependence of EFG might be changed in nanocrystalline non-cubic metals as well. Nanocrystalline Indium has been prepared with different particle sizes by the method of electrochemical deposition. The temperature dependence of the EFG as a function of different particles sizes (11 nm, 12, nm, 27 nm, as determined by TEM) was investigated in the temperature range of 20-300 K using the perturbed $\gamma\gamma$-angular correlation technique (PAC). The data show that the temperature dependence of the EFG in nanokristalline In still follows a $T^{3/2}$ dependence. However, the coupling constant $\nu_Q(0)$, extrapolated to zero temperature, and the slope B, quantifying the $T^{3/2}$, relation are changed compared to the respective values of the bulk material. Both parameters obviously depend on the grain size of nanocrystalline In. From the analysis of the data it is concluded that the observed changes of the EFG can completely be explained by changes of the lattice constants.
Supported by the DFG within the SFB 277.

MM 19.3 Sa 11:30 TU H111

Recrystallization effect in giant magneto resistance (GMR) systems during annealing — •Vitaliy Vovk and Guido Schmitz — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Strasse 10, D-48149 Münster, Germany

The long-term thermal stability of giant magneto resistance (GMR) multi-layer systems is a key issue regarding their technical application. In Py/Cu and Py/Cu/Co layer systems a recrystallization is induced by annealing at temperatures in the range of 400-500°C, which leads to a transformation of the crystallographic orientation from a [111] to a [200] wire texture. The main aim is to show that this recrystallization is triggered by the minimization of the elastic energy that is caused by the lattice mismatch between the thin film layers. Therefore, the PyCu-system is chosen for the study, since the lattice mismatch can be controlled by the concentration of iron in Py (mixture of Ni and Fe). Beside, the influence of other factors like sputtering rate, Ar-gas pressure, and magnetic fields applied during sputtering is investigated and their influence on the microstructure is discussed.

MM 19.4 Sa 11:45 TU H111

selective synthesis of nano-meter-sized clusters: size and structure determination — •M. Suleiman[1], C. Borchers[1], M. Guerdane[1], N. M. Jisrawi[2], M. T. Reetz[3], R. Kirchheim[1], H. Teichler[1], and A. Pundt[1] — [1]Institute fuer Materialphysik, Uni. Goettingen — [2]Department of Physics, Birzeit University, Palestine — [3]Max-Planck-Institut fuer Kohlenforschung, Muelheim

Using electrochemical technique [[1]] we will show that not only the clusters size can be selectively prepared but also the structure. Palladium clusters are prepared in a simple two-electrode cell in which surfactant is used as electrolyte and stabiliser. The obtained cluster sizes depend on the preparation parameters, such as: current density, temperature, type of solvent and distance between the electrodes. Using XRD and TEM analysis show a narrow size distribution ((± 0.5 nm)). The cluster size is evaluated from the XRD data and TEM images. It will be shown that a Fourier transform of the XRD pattern gives a fairly accurate value of the cluster size. XRD and HREM analysis revealed that the structure of the Pd clusters is size dependent. The critical size for the structural transition from icosahedral to cubic structure was found to be 4.8 nm. This result is in good agreement with the critical size value obtained from MD-simulation for a model Pd clusters [[2]]. First results on preparing Ni, Co and core shell clusters using this electrochemical technique will be presented.
This work is supported by the DFG via SFB 602 [[1]] M. T. Reetz, W. Helbig, J. Am. Chem. Soc., 11 ((1994)) 7401 [[2]] N. M. Jisrawi, A. Pundt, M. Guerdane, H. Teichler accepted in Acta Mater.

MM 19.5 Sa 12:00 TU H111

Nanoparticles of intermetallic phases extracted from Ni-base alloys — •Giancarlo Pigozzi, Debashis Mukherji, and Gernot Kostorz — ETH Zürich, Institute of Applied Physics, CH-8093 Zürich, Switzerland

Single crystalline nanoparticles of Ni alumides and silicides have been produced by an electrochemical process based on selective dissolution of the matrix phase of a two-phase alloy containing an intermetallic precipitate phase. The precipitates were grown to less than 50 nm mean size by an isothermal aging treatment. Electrochemical potentiometric experiments were performed to determine the appropriate process parameters for the extraction of the nanoparticles. The collection of nanoparticles after the extraction poses a serious challenge. Ultrasonic vibration and centrifuge are employed for separating the nanoparticles from the sample surface and from the liquid bath. Results are presented on characterisation of the microstructure of the alloy and the extracted particles by SEM, TEM, and XRD. The composition control and the control of homogeneity of multicomponent nanoparticles is relatively easy, in this technique. The process is demonstrated presently only at the laboratory scale and even at this scale, only a tiny amount of material (in mg) is obtained when the particles are less than 50 nm in size. Work is in progress to increase the yield.

MM 19.6 Sa 12:15 TU H111

Phase Formation During Solidification of a Ti-Based, In-Situ, Nanostructured Matrix Composite — •Thomas Woodcock[1], Germán Alcalá[1], Sonia Mato[1], Wolfgang Löser[1], Annett Gebert[1], Jürgen Eckert[2], and Ludwig Schultz[1] — [1]IFW Dresden, P.O. Box 270016, 01171 Dresden, Germany — [2]TU Darmstadt, FB Material- und Geowissenschaften, FG Physikalische Metallkunde, Petersenstraße 23, 64287 Darmstadt, Germany

Ti-based, in-situ formed, nanostructured matrix composites such as Ti60Cu14Ni12Sn4Ta10 combine the high yield stress of nanocrystalline materials with the plasticity and toughness of conventional alloys. The remarkable mechanical properties arise from a microstructure, formed after Cu-mould casting, which consists of micron-scale dendrites of β-Ti solid solution in a nanoscale eutectic matrix. Detailed characterisation of the phases in the eutectic matrix has shown that they are β-Ti solid solution and the intermetallic NiTi which contains significant amounts of Cu in solution. Comparison with the ternary Ti-Cu-Ni system established that

the eutectic in the composite forming alloy is metastable due to kinetic exclusion of the equilibrium phase at such compositions, CuTi2. The understanding of the solidifcation processes of such materials is important for alloy development and may lead to new materials suitable for a wider range of potential applications.

MM 20 Intermetallische Phasen I

Zeit: Samstag 09:15–10:30 Raum: TU H2038

MM 20.1 Sa 09:15 TU H2038

Mechanical Spectroscopy of Fe-Al alloys with Al concentrations up to 26 at.%. — •A. Strahl[1], S.B. Golovina[2], I.S. Golovin[2], and H. Neuhäuser[1] — [1]TU-BS, Institut für Metallphysik u. Nukleare Festkörperphysik, D-38106 Braunschweig — [2]TU-BS, Institut für Werkstoffe, D-38106 Braunschweig

Temperature and time dependent internal friction (mechanical spectroscopy) of quenched Fe-Al-C alloys has been measured monitoring the Snoek-type relaxation (jumps of interstitial carbon atoms) in dependence of Al concentration. With an increase of Al substitutes in iron, the Snoek type peak changes its shape in a few steps. In the range 3-8 at.% Al in iron the peak is clearly composed of two Debye-type peaks: the peak at lower temperature corresponds to the original Snoek peak; the peak at higher temperature is caused by jumps of carbon atoms on places with nearby Al atoms. Above a critical Al concentration the original Snoek peak practically vanishes: in that case the surrounding of a C-atom is changed from Fe atoms to a random or ordered mixture of Fe and Al atoms, increasing the carbon hopping potential, shifting the Snoek-type relaxation to higher temperatures, and increasing the peak widths; such a peak is recorded in intermetallic compounds Fe_3Al.

By isothermal annealing experiments at selected temperatures around the observed peaks the long-term kinetics of carbon jumps has been followed in some detail to evaluate parameters of the process of carbon atoms removal from the interstitial solid solution. The observation of two relaxation rates associated with the decrease of Snoek-type peaks in Fe-Al-C alloys corresponds to nucleation and growth of carbides.

MM 20.2 Sa 09:30 TU H2038

Mechanical spectroscopy of high pressure torsion (HPT) deformed Fe_3Al based alloys — •T.S. Pavlova[1,2], I.S. Golovin[2], H.-R. Sinning[2], and R.Z. Valiev[3] — [1]Physics of Metals Department of Tula State University, Lenin ave. 90, Tula, Russia — [2]TU Braunschweig, Institut fuer Werkstoffe, Langer Kamp 8, D-38106 Braunschweig — [3]Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, Russia

The method of mechanical spectroscopy (especially internal friction measurements) is known as an effective tool for studying dislocation behaviour in deformed metals. However, for brittle intermetallic compounds like Fe_3Al, a problem is that deformation at room temperature is hardly possible by ordinary methods but requires special techniques like, for instance, high pressure torsion (HPT).

Several internal friction peaks were distinguished in HPT Fe_3Al-based alloys. Most of them are analogous to those found in deformed and irradiated pure iron, where they are known to be caused by dislocations. In HPT Fe-Al specimens, these peaks are significantly reduced already by moderate heat treatments, including even the unavoidable tempering during the measurements themselves. It is notable that using these internal friction peaks, earlier stages of annealing processes in HTP materials can be detected than by other methods, which show annealing effects only at higher temperatures. Preliminary interpretations of these peaks will be presented.

MM 20.3 Sa 09:45 TU H2038

Einfluss der Wärmebehandlung auf die Fernordnung und die magnetischen Eigenschaften von dünnen Filmen aus FePd — •Chaisak Issro[1], Wolfgang Püschl[1], Wolfgang Pfeiler[1], Peter F. Rogl[2], William A. Soffa[3], Rafal Kozubski[4] und Veronique Pierron-Bohnes[5] — [1]Inst. f. Materialphysik, Universität Wien — [2]Inst. f. Phys. Chemie, Universität Wien — [3]Dept. of Mat. Sci. & Eng., Univ. of Pittsburgh — [4]M. Smoluchowski Inst. of Physics, Jagellonian Univ. Cracow — [5]Inst. Phys. & Chim. Materiaux de Strasbourg

Dünne Filme aus FePd wurden auf Si gesputtert und auf MgO epitaktisch aufgebracht. Zum Vergleich wurde die Ordnungseinstellung einer anfangs ungeordneten, kaltgewalzten Folie während einer isochronen Wärmebehandlung mit Röntgenbeugung, Restwiderstandsmessungen und ihrem magnetischen Verhalten verfolgt. Der auf Si-Substrat aufgesputterte Film ist zuerst völlig ungeordnet. Bei der anschließenden Auslagerung ordnet der Film in $L1_0$-Struktur, wobei alle Varianten geordneter Domänen entstehen (Magnetisierungskurven). Die epitaktischen Filme sind sofort hoch geordnet, nahezu einkristallin (c-Achse normal zur Filmoberfläche) und magnetisch anisotrop. Ab 500 K beginnen sich die geordneten Domänen mit ihrer c-Achse in die Filmebene zu drehen. Dieser überraschende Effekt stimmt mit jüngsten MC-Simulationen der Ordnungskinetik in sehr dünnen FePt Schichten (10 Atomlagen) überein.

MM 20.4 Sa 10:00 TU H2038

Long-periodic superlattices in Cu-rich Cu-Pd alloys - an ab-initio study — •S. Bärthlein[1], G.L.W. Hart[2], A. Zunger[3], and S. Müller[1] — [1]Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Department of Physics and Astronomy, Northern Arizona University, Flagstaff, Arizona 86011-6010 — [3]National Renewable Energy Laboratory, Golden, Colorado 80401

Beside the well-known L12-phase, Cu-rich Cu-Pd alloys form one- and two-dimensional long-periodic superlattices (LPS). Combining total-energy DFT calculations, a mixed-space cluster-expansion (CE) and genetic algorithms [1], we construct effective multibody interactions, allowing for a detailed study of the structure and stability of these LPS-phases. In good agreement with experiment, at 25% Pd a subtle hierarchy of LPS-structures is found with the so-called LPS3-structure as T=0K ground state, *not* just being an entropically stabilized feature. With the help of Monte-Carlo simulations, phase transition temperatures and short-range order behaviour (SRO) are predicted. Hereby, the SRO-pattern of the LPS-phase shows a four-fold peak-splitting at $\langle 110 \rangle$ and a two-fold one at $\langle 100 \rangle$, allowing for a determination of the Fermi-vector. The results are in excellent agreement with experimental data. (Supported by DFG.)

[1] G.L.W. Hart et al., submitted (2004)

MM 20.5 Sa 10:15 TU H2038

Characterization of Cu/Sn and Cu/SnPb solder reaction — •Jens Görlich and Guido Schmitz — Institut für Materialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

Development of leadfree solders and a further size reduction in electronic devices require a better understanding of physical mechanisms during soldering. Diffusion paths, kinetic processes and - especially for microdevices - the unfavorable fast growth of the non planar intermetallic Cu_6Sn_5 layer during the interreaction between solid Cu and liquid tin-lead or pure liquid tin solder have been investigated. SEM analyses revealed a time dependence of the scallop-like Cu_6Sn_5 intermetllic layer of $R \sim t^{1/3}$. The interfaces between Cu and the solder were analysed by HREM and EELS and the wetting angles for pure tin and tin-lead solder were determined. The growth of the scallop like structure is controlled by grain boundary diffusion across the existing Cu_6Sn_5 layer. Nevertheless, the observed process may be still described by a recent model [1], which assumes the transport through channel of liquid solder. Furthermore, the influence of a sputter-deposited Cu_6Sn_5 base metallization was investigated. The results will be discussed in view of the technologically desired limitation of the fast growth of Cu_6Sn_5.

[1] A.M. Gusak, Phys. Rev. B 66, 115403 (2002)

MM 21 Intermetallische Phasen II

Zeit: Samstag 11:00–12:15 Raum: TU H2038

MM 21.1 Sa 11:00 TU H2038

Microstructural characterization of Inconel 706 alloy — •V. Kindrachuk[1], N. Wanderka[1], J. Banhart[1], D. Del. Genovese[2], and J. Rösler[2] — [1]Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany — [2]Technical University Braunschweig, D-38106 Braunschweig, Germany

Inconel 706 is a wrought Ni-Fe base superalloy which is used for applications at service temperatures up to 600°C. It develops its good mechanical properties by precipitation of intermetallic phases γ' ($L1_2$ structure) and γ" (DO_{22} structure) in the austenitic γ matrix. Microstructure evolution was studied after ageing times of 750 h and 5000 h at 750°C. Characterization of the precipitates and of the matrix was carried out by three-dimensional atom probe tomography and by transmission electron microscopy. The modified stabilization treatment produces individual γ' and γ" precipitates and γ'-γ" co-precipitates with average sizes of about 20 nm which are oriented parallel to the $< 001 >$ lattice direction of the γ matrix. There were also observed much bigger individual γ" precipitates with sizes above 50 nm. In addition η precipitates forming at the grain boundaries are detected. The matrix volume fraction after MST is 89 %. During heat treatment at 750°C the small precipitates growth first and are then transformed to η phase. The γ"-phase growths into needles of about 500 nm size. After 5000 h of ageing only one type of precipitates remains, namely η plates embedded into the matrix. The matrix is more enriched in Ni and depleted in Fe as compared with the preceding treatment. The volume fraction of the matrix is close to 93 %.

MM 21.2 Sa 11:15 TU H2038

Variation of Lattice Distortion of Gamma Prime Phase in Creep-deformed Single Crystal Superalloy SC16 with Temperature — •Weye Chen[1], Nora Darowski[2], Ivo Zizak[2], Gerhard Schumacher[2], Helmut Klingelhöffer[3], and Wolfgang Neumann[1] — [1]Humboldt University Berlin, Institute of Physics — [2]Hahn-Meitner-Institute Berlin , Structure and Dynamics — [3]Federal Institute of Materials Research and Testing, Berlin

The lattice distortion of gamma prime precipitates in creep-deformed single crystal superalloy SC16 was investigated by means of high resolution X-ray diffraction technique using synchrotron radiation. The specimens were deformed at 1223 K and 150 MPa to a creep strain of 0.5 temperature. Variations in FWHM can in principle be caused by changes in the size of gamma prime precipitates and by changes in the lattice distortion with temperature. A detailed analysis with respect to the above mentioned aspects led to the conclusion that the effect observed in the present study is essentially caused by temperature-dependent redistribution of internal lattice distortion between gamma prime precipitates and gamma matrix, rather than by changes in precipitate size.

Work supported by DFG (Neu 646/5-3 and Schu 1254/3-4)

MM 21.3 Sa 11:30 TU H2038

First-principles prediction of novel ground state structures for the binary systems made of Nb, Ta, Mo, W* — •Volker Blum[1] and Alex Zunger[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]National Renewable Energy Laboratory, Golden, Colorado 80401, USA

The refractory metals Nb, Ta, Mo, and W are the most prominent body-centered cubic transition metals in the periodic system of elements. While the measured mixing enthalpies are negative, implying the existence of some long-range ordered binary crystal structures, the phase diagrams, restricted so far to high-temperature measurements, have revealed only random alloys at high T. It was previously guessed that the ordered structures are ordinary B2 (CsCl type) or $D0_3$ (BiF_3 type), but in principle could be any of the infinite number of other configurations. Combining DFT calculated energies of O(50) configurations for each binary with a "Mixed Basis Cluster Expansion" whose interaction types are chosen by a genetic algorithm search, we derive the energy for *any* bcc configuration. This (Ising-like) functional is then searched to find T=0 ground state structures, and to compute (via Monte Carlo) finite T thermodynamics. The ground states reflect directly the complexity of the underlying interatomic interactions, with the observed absence of high-temperature ordered phases as a consequence. We also predict atomic short-range order in the solid solutions at finite T.

*Work performed at NREL under DOE-BES support.

MM 21.4 Sa 11:45 TU H2038

On the broken-bond model and the pair-potential modelling of alloy surfaces — •Ralf Drautz[1,2] and Manfred Fähnle[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Department of Materials, University of Oxford, OX1 3PH, UK

The existence of a surface breaks the symmetry of the bulk material leading in general to an ordering behaviour at the surface which is different from the one of the bulk. We discuss the theoretical modelling of this situation with the cluster-expansion (CE) method [1] and with the many-body potential expansion [2], and we apply these calculational techniques to the system $Ni_{90}Al_{10}(110)$ [1]. It is shown that a broken-bond model which discards the contributions to the CE of clusters with bonds pointing out of the surface and assumes bulk values for the contributions of the remaining clusters may fail badly to describe surface segregation and ordering. The tendency of a minority atom to segregate to the surface of a diluted binary alloy is discussed by use of pair potentials. It is shown that perfectly transferable and hence environment-independent pair potentials [2] in general cannot describe the situation adequately.

[1] R. Drautz, H. Reichert, M. Fähnle, H. Dosch, and J. M. Sanchez, Phys. Rev. Lett. **87**, 236102 (2001)
[2] R. Drautz, M. Fähnle, and J. M. Sanchez, J. Phys.: Condensed Matter **16**, 3843 (2004)

MM 21.5 Sa 12:00 TU H2038

Solidification of Undercooled Intermetallic Forming Systems — •Hamid Assadi[1,2] and Dieter M. Herlach[1] — [1]DLR, Institut für Raumsimulation, 51147 Köln — [2]On leave from: Tarbiat Modarres University, Tehran, Iran

Intermetallics exhibit unique solidification behaviour due to their chemical long-range order. This inclues, for instance, generally slow solidification kinetics, and in some cases, a characteristically sharp change of slope in the corresponding relation between crystal growth velocity and undercooling. The present work uses a phase-field approach to illustrate this behaviour, and further to predict an entire microstructure in an intermetallic forming system. The phase field model is derived from a thermodyanamic formulation, and is assessed qualitatively against the sharp-interface theory of disorder trapping by Boettinger and Aziz (Acta Metall. 1989). A quantitative assessment of the model is provided with respect to the measured growth velocity - undercooling data for various Ni-Al alloys, obtained from electromagnetic levitation experiments.

(Support by the Alexander von Humboldt-Foundation is gratefully acknowledged.)

MM 22 Hauptvortrag Andreas Schreyer

Zeit: Samstag 14:00–14:30 Raum: TU H1058

Hauptvortrag MM 22.1 Sa 14:00 TU H1058

Engineering Materials Research with Neutrons and Photons: Contributions to better Lightweight Structures — •Andreas Schreyer — GKSS Forschungszentrum GmbH, Max Planck Str. 1, 21502 Geesthacht

For the development and optimization of lightweight structural materials characterization methods are needed which provide an intimate knowledge of their micro- and nanostructure. Neutrons and photons from synchrotron radiation sources can provide information e.g. on strains, textures, precipitates, pores and cracks in a destruction-free way. In this talk a number of examples from the ongoing development of TiAL and Mg alloys and parts as well as on welding technologies will be presented, where neutrons and photons were able to make an important contribution using scattering or tomographic techniques. Specifically, the complementarity of both probes will be highlighted.

MM 23 Phasenumwandlung III

Zeit: Samstag 14:45–16:30 Raum: TU H1058

MM 23.1 Sa 14:45 TU H1058

Phase-field study of the cellular bifurcation in dilute binary alloys — •Mathis Plapp and Esteban Meca — Laboratoire PMC, Ecole Polytechnique, 91128 Palaiseau, Frankreich

In the directional solidification of dilute binary alloys, a planar interface becomes unstable at a critical speed of the solidification front that depends on the alloy concentration and the applied temperature gradient. We investigate the microstructures that form closely above this instability threshold using phase-field simulations in both two and three dimensions. In particular, we study the so-called 'node' or 'pox' structures that consist of regular hexagonal arrays of 'holes' (local depressions of the solidification front) and compare their properties to the ones of the well-known hexagonal cell patterns. The results are compared to the predictions of weakly nonlinear amplitude expansions as well as to experimental findings.

MM 23.2 Sa 15:00 TU H1058

In-situ Determination of Phase Selection Sequences and Short-Range Order in Undercooled Ti-Fe-Si-O Melts — •Oliver Heinen, Dirk Holland-Moritz, Thomas Volkmann, Jörn Strohmenger, and Dieter M. Herlach — DLR, Inst. für Raumsimulation, D-51170 Köln

The alloy system Ti-Fe-Si-O shows a great variety of complex stable and metastable phases. Depending on composition and undercooling different solidification pathways are found. The large number of alloy phases in Ti-Fe-Si-O leads to a strong competition of phase selection during rapid solidification of undercooled melts. In order to determine the phase formation sequence as function of composition and to examine possible dependencies on the short-range order (SRO) of the undercooled liquid, in situ investigations of SRO and solidification pathways were performed. The containerless processing technique of electromagnetic levitation was combined with energy dispersive diffraction of synchrotron radiation at the European Synchrotron Radiation Facility. This enables us to directly determine the crystal structure of the solid phases formed during rapid solidification and to study the SRO of the liquid in the same experiment. Depending on the undercooling different solidification sequences were found. In addition the SRO was also investigated using neutron diffraction at the Institut Laue-Langevin. The complementary results on the SRO obtained by neutron and x-ray diffraction are discussed in terms of the effects of topological and chemical SRO.

This work was financially supported by DFG under contract No. Ho1942/4 and by ESRF and ILL.

MM 23.3 Sa 15:15 TU H1058

In-situ Determination of Phase Formation in Undercooled Nd-Fe-B-melts – Identification of a Metastable Phase with Synchrotron Radiation — •Jörn Strohmenger[1], Thomas Volkmann[1], Jianrong Gao[2], Sven Reutzel[3], Dirk Holland-Moritz[1], Oliver Heinen[1], and Dieter M. Herlach[1] — [1]Institute of Space Simulation, German Aerospace Center (DLR), D-51170 Cologne — [2]Key Lab of Electromagnetic Processing of Materials (EMP), Northeastern University, Shenyang 110004, China — [3]Institute of Experimental Physics IV, Ruhr-University Bochum, D-44780 Bochum

Nd-Fe-B alloys are of special interest due to the excellent hardmagnetic properties of the intermetallic compound $Nd_2Fe_{14}B_1$ (Φ-Phase). Competitive crystallisation of stable and metastable phases in undercooled Nd-Fe-B melts was investigated using electromagnetic levitation combined with in-situ X-ray diffraction experiments at the ESRF. Under equilibrium conditions for alloys near the stoichiometric composition the Φ-phase is formed by a peritectic reaction from pro-peritectic γ-Fe. For Nd-contents between 10 and 18at% at the ratio $\frac{\mathrm{Nd}}{\mathrm{B}} = \frac{2}{1}$ it is shown that the crystallization of primary phase is affected by undercooling, e.g a metastable phase can be directly observed which initiates the formation of the Φ-phase. It can be identified as a ternary extension of the rhombohedral Nd_2Fe_{17} phase being stable in binary Nd-Fe alloys. A phase selection diagram showing the different solidification pathways as a function of undercooling and alloy composition will be analysed within theories of nucleation and crystal growth. This work was supported by DFG under contract No. HE1601/14.

MM 23.4 Sa 15:30 TU H1058

Phase-field simulations of solidification structures in multicomponent (Ni-Cu-Cr) and multiphase (Al-Cu) alloys — •Denis Danilov and Britta Nestler — Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Phase transformations in multicomponent and multiphase (e.g. eutectic) systems play a major role during solidification processes of a variety of alloys. Using a general phase-field model we investigate growth microstructures and their dependence on solidification conditions in such systems. In ternary Ni-Cu-Cr alloy a morphological transition from dendritic to globular growth is found by varying the alloy composition at a fixed underccoling. The dependence of the growth velocity and of the impurity segregation in the solid phase on the composition is analyzed and indicates a smooth type of transition between the dendritic and globular structures. The stability of lamellar eutectic structure in Al-Cu alloy is investigated and two possible types (regular and oscillatory) of the growth structures have been found depending on the lamellar spacing and on the off-eutectic composition. The work was supported by DFG under project No. Ne 882/2.

MM 23.5 Sa 15:45 TU H1058

Die Entstehung dendritischer Mikrostruktur in einem metallischen Glaskomposit — Y.-L. Huang[1], •T. Niermann[1], M. Seibt[1], S. Schneider[1], B. Nestler[2] und D. Danilov[2] — [1]IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Fachhochschule Karlsruhe, Moltkestrasse 30, 36133 Karlsruhe

Wir präsentieren die Ergebnisse unserer Untersuchungen der Mikrostruktur eines massiven Glas-Komposits. Die Untersuchungen wurden mittels Transmissionselektronenmikroskopie (TEM), energiedispersiver Röntgenanalyse (EDX) und Elektronenenergieverlustspektroskopie (EELS) durchgeführt. Dabei beobachten wir eine in der Glasmatrix eingebettete dendritische BCC-Phase, die während der Abkühlung einer Schmelze der Zusammensetzung $Zr_{59}Ti_{14}Nb_5Cu_7Ni_6Be_{12}$ entsteht. Die Verteilungen der Elemente (Zr, Ti, Nb, Cu, Ni und Be) im Volumen der beiden Phasen sowie an der Grenzfläche zwischen Dendrit und Matrix konnten experimentell bestimmt werden. Die experimentellen Ergebnisse werden mit numerisch simulierten Konzentrationprofilen verglichen. Zur Durchführung der Simulationen des dendritischen Wachstums wird ein pseudo-ternäres Phasendiagramm mit 3 Komponenten A=(Zr,Ti,Nb), B=(Ni,Cu) und Be betrachtet. Wir verwenden eine allgemeine Formulierung eines multikomponentigen Phasenfeldmodells zur Beschreibung des Phasenübergangs von der Schmelze zum Dendriten.

MM 23.6 Sa 16:00 TU H1058

Solidification of Undercooled Si, Si-Co and Si-Ge Melts — •C. Panofen[1], R.P. Liu[2], and D.M. Herlach[1] — [1]DLR Köln, Institut für Raumsimulation — [2]Yanshan University, Qinhuangdao, China

We undercooled and solidified pure Si, dilute Si-Co and Si-Ge melts in a high purity environment containerlessly by electromagnetic and electrostatic levitation techniques. Without surrounding crucible walls and thus reducing heterogeneous nucleation sites we achieved large melt undercoolings of up to 330K.

Crystallization at the desired undercooling was initiated by triggering with a silicon wafer. The velocity of the solidification front as a function of undercooling was directly determined with a high speed camera.

We analyzed the growth behavior within current theories of crystal growth in undercooled melts. Special emphasis was placed to a microstructure transition from faceted to dendritic growth. The results of the growth measurements were correlated to microstructure formation upon undercooling prior to solidification.

This work is funded by the Sino-German Science Center, Beijing, and DFG under contract number HE-1601/16-1

MM 23.7 Sa 16:15 TU H1058

SANS Untersuchungen an unterkühlte Schmelze — •O. Perroud[1], A. Wiedenmann[1], D. Holland-Moritz[2] und D. Herlach[2] — [1]Hahn-Meitner Institut Berlin, Glienickerstr.100, D-14109 Berlin — [2]DLR, Institut für Raumsimulation, Linder Höhe, D-51147 Köln

Über die Natur möglicher Nahordnung in unterkühlten Schmelzen ist bisher wenig bekannt. Theoretische Arbeiten [1] postulierten eine iko-

saedrische Nahordnung, die kürzlich durch eleastische Neutronenstreuexperimente im Großwinkelbereich bestätigt wurde [2]. Wir berichten über Untersuchungen an unterkühlten Schmelzen von reinem Ni und von Cu-Co Legierungen mit Hilfe der Neutronen-Kleinwinkelstreuung. Die Proben wurden in einem elektromagnetischen Levitationsofen geschmolzen und in-situ auf dem SANS Instrument V4 am HMI, Berlin untersucht. Durch den tiegelfreien Prozess der Schmelze unter hochreinen Bedingungen wurde heterogene Keimbildung unterdrückt, wodurch Unterkühlungen bis zu 300°C erreicht wurden. Im Verlauf der Unterkühlung tritt neben der inkohärenten Flüssigkeitsstreuung ein Kleinwinkel-Streusignal auf, das auf Dichte-Fluktuationen im Nanometerbereich hindeutet. [1] F.C. Frank, R. Soc. A215(1952) 43. [2] T. Schenk, D. Holland Moritz, V. Simonet, R. Bellissent and D.M. Herlach, Phys. Rev. Lett. 89 (2002) 075507.

MM 24 Nanoskalige Materialien III

Zeit: Samstag 14:45–16:00 Raum: TU H111

MM 24.1 Sa 14:45 TU H111

Computersimulation der Kondensation von Nanopartikeln aus der Gasphase — •Ralf Meyer — Département de physique, Université de Montréal, C.P. 6128 succ. Centre-Ville, Montréal (Québec) H3C 3J7, Kanada

Die Bildung von Ni Nanopartikeln aus der Gasphase wird mit Hilfe von Molekulardynamik-Simulationen untersucht. Diese Simulationen zeigen, wie sich zunächst sehr heiße flüssige Nickeltröpfchen bilden, die im weiteren Verlauf kristallisieren und schließlich zu größeren Teilchen agglomerieren. Die strukturellen Eigenschaften der resultierenden Teilchen sind denen von experimentell hergestellten Nickel Nanopartikeln sehr ähnlich. Die Kühlung in den Simulationen erfolgt durch die Wechselwirkung der Nickelteilchen mit den Atomen eines dünnen Argongases. Eine Analyse der Aufteilung der kinetischen Energie zeigt, dass dabei die verschiedenen Freiheitsgrade des Systems unterschiedlich schnell thermalisieren. Die in den Translations- und Rotationsfreiheitsgraden der Teilchen gespeicherte kinetische Energie nimmt deutlich langsamer ab die Energie in den Schwingungsfreiheitsgraden der Teilchen. Insbesondere die überproportional hohe Rotationsenergie könnte dabei einen Einfluß auf die Struktur der entstehenden Teilchen haben.

MM 24.2 Sa 15:00 TU H111

Modeling of the ECAP process: Misorientation evolution — •Ralph Jörg Hellmig[1], Hyoung Seop Kim[2], and Juri Estrin[1] — [1]Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678 Clausthal-Zellerfeld — [2]Dept. of Metallurgical. Eng., Chungnam National University, Daejeon, 305-764, Korea

Using Equal Channel Angular Pressing (ECAP) an ultrafine grained microstructure can be achieved. It has been demonstrated that FEM calculations based on a dislocation density related constitutive model are a suitable method to describe the structure refinement as well as the evolution of mechanical properties and overall texture [1,2]. So far, the evolution of the average misorientation between neigbouring dislocation cells was not included in this model description. A simple extension based on experimental evidences introduced in the FEM code allows to trace the evolution of the average misorientation angle. Results of modeling will be compared with experimental data.
[1] S.C. Baik, R.J. Hellmig, Y. Estrin, H.S. Kim; Z. Metallkd. 94 (2003) 754.
[2] S.C. Baik, Y. Estrin, R.J. Hellmig, H.T. Jeong, H.G. Brokmeier, H.S. Kim; Z. Metallkd. 94 (2003) 1189.

MM 24.3 Sa 15:15 TU H111

Designing tools for ECAP processing — •Mikhail V. Popov, Torbjørn Lamark, Ralph Jörg Hellmig, and Juri Estrin — Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678 Clausthal-Zellerfeld

In recent years Equal Channel Angular Pressing (ECAP) became one of the most important methods for the production of ultrafine grained materials. General ECAP tools are simple in design, but to have really good processing conditions to achieve homogeneous microstructures more advanced tools including features like backpressure or even sliding walls are necessary. In this talk, an introduction on the critical parameters of ECAP processing will be given followed by a discussion of possible solutions for obtaining high performance ECAP equipment.

MM 24.4 Sa 15:30 TU H111

Molecular dynamics investigation of the coalescence of iron nanoparticles — •Norbert Lümmen and Thomas Kraska — Universität zu Köln, Institut für Physikalische Chemie, Luxemburger Str. 116, D-50939 Köln

Coalescence is an important process over the course of the formation of nanoparticles. It significantly influences the properties of the resulting particles. In this work we have investigated the coalescence of iron nanoparticles in the gas phase. Argon has been added in order to reproduce the experimental situation in an inert gas aggregation source (IGA). The heat generated during the coalescence is removed from the system via the inert gas atoms. For the calculation of the interaction between the iron atoms a further development of the embedded atom method for iron taken from the literature has been employed.

The investigation shows that the coalescence of structured clusters evolves via three steps. Each of these steps happens on a different time scale and at different degree of heat exchange with the inert gas. So far such investigations have been performed without an inert gas and therefore the cooling down of the particles during the coalescence has been omitted.

MM 24.5 Sa 15:45 TU H111

Highly ordered nanoparticle arrays with tunable shape, size and spacing — •Yong Lei, Jörg Weissmüller, and Gerhard Wilde — Institute of Nanotechnology, Research Center Karlsruhe, P.O.Box 3640, D-76021 Karlsruhe, Germany

We report an approach to fabricate highly ordered semiconductor or metal nanoparticle arrays with controllable shape, size and spacing. Nanometer-sized discs, hemispheres, hemi-ellipsoids, and conical morphologies have successfully been obtained. The nanoparticle arrays are fabricated on Si or Si/SiO_2 substrates, using ultra-thin alumina membranes as evaporation masks. The shapes and the sizes of the nanoparticles are adjusted by changing the aspect ratio of the apertures of the nanostructured masks and the amount of material deposited through the nanoporous membranes. The size of the arrayed nanoparticles can be adjusted from 10 to 200 nm. The nanoparticle arrays reported here have been applied in some areas, including field emission and electronic devices. In addition, the nanoparticle arrays are well-suited for investigations concerning size-dependent phenomena due to their extremely narrow size distribution.

MM 25 Material Design

Zeit: Samstag 14:45–16:30 Raum: TU H2038

MM 25.1 Sa 14:45 TU H2038

Consolidation Process during Diffusion Bonding in Continuous Al2O3 Fiber-reinforced NiAl Composites — •Hao Chen, Weiping Hu, Yunlong Zhong, and Günter Gottstein — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen, 52056, Aachen, Germany

A theoretical model for solid-state diffusion bonding during the consolidation process of continuous Al2O3 fiber reinforced NiAl composites has been presented. The aim of which was to evaluate the operated mechanisms for consolidation and to determine the optimal hot pressing parameters (time, temperature, pressure). It was found that plastic deformation caused by creep was dominant mechanism in the consolidation process at high temperatures and high pressures. Only in the final collapse of the porosities, the diffusion mechanisms (surface diffusion, volume diffusion and grain boundary diffusion) played a relative important role. The effects of fiber volume fraction and the arrangement of the

matrix-coated fibers were also analyzed. Different dense composites were fabricated according to the predicted processing parameters, and good agreement between experimental results and predictions from the model was achieved.

MM 25.2 Sa 15:00 TU H2038

Thermomechanische Eigenschaften interpenetrierender Graphit / Aluminium-Verbundwerkstoffe — •Thomas Etter und Peter J. Uggowitzer — Laboratorium für Metallphysik und Technologie, ETH Zürich, CH-8093 Zürich, Schweiz

Durch die Infiltration von isotropen mikroporösen Graphitvorformen (15 Vol.% Porosität) mit AlSi-Legierungen wurden Graphit/Aluminium-Verbundwerkstoffe mit einem Durchdringungsgefüge hergestellt. In diesem interpenetrierenden Mehrphasenwerkstoff bildet jede Phase ein dreidimensionales Netzwerk aus, das zur makroskopischen Werkstoffeigenschaft des Verbundwerkstoffes beiträgt. Leichtmetallinfiltrierte Graphite könnten in Zukunft herkömmliche Al-Legierungen als Kolbenwerkstoffe in Verbrennungsmotoren konkurrieren. Durch die Leichtmetallinfiltration kann die 4-Punkt-Biegebruchfestigkeit von 60 MPa auf 120 MPa verdoppelt werden. Diese Festigkeitserhöhung ist hauptsächlich auf eine Erhöhung der Bruchzähigkeit durch plastische Verformung des duktilen Aluminiums zurückzuführen. Mit diesem Ansatz kann auch erklärt werden, wieso diese C/Al-Verbundwerkstoffe bei 300°C keinen Festigkeitsabfall gegenüber Raumtemperatur zeigen. Um die Anfälligkeit der Verbundwerkstoffe auf thermische Wechsellasten zu untersuchen, wurden die mechanischen Eigenschaften sowohl direkt nach der Herstellung als auch nach 1000 thermischen Zyklen (zwischen Raumtemperatur und 300°C) bestimmt. Je nach Legierungszusammensetzung können Ausscheidungsvorgänge in der Metallphase zu einer leicht verringerten Bruchzähigkeit bzw. Festigkeit nach dem thermischen Zyklieren führen.

MM 25.3 Sa 15:15 TU H2038

Assembly and properties of single- and multilayer topologically interlocked structures made from cubic elements — •Stephan schaare[1], Juri Estrin[1], Arcady Dyskin[2], Elena Pasternak[2], and Han Chuan Khor[2] — [1]Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678 Clausthal-Zellerfeld — [2]School of Civil and Resource Engineering, The University of Western Australia, 35 Stirling Highway, Crawley, WA 6009, Australia

Topological interlocking is a novel concept for designing materials, in which elements of certain geometries are assembled in a special way to support each other and form an integral structure without the need for connectors or a binder phase. Geometric bodies which allow such an assembly into topologically interlocked structures are the five platonic bodies. We present assemblies of single- and multilayer structures of cube shaped elements along with the results of mechanical tests done on these structures, *viz.* quasistatic point loading and impact loading tests. Different kinds of materials and surface treatments were used for the cube elements. The results show that the properties of the structures strongly depend on the material and the surface condition of the individual elements, as well as on the lateral loading of the structure. The impact tests reveal enhanced energy absorption by the topologically interlocked structures. Also an unusual mechanical response in point loading tests was observed, in which the structures show a negative stiffness. These properties underpin both practical applications and theoretical significance of these novel structures.

MM 25.4 Sa 15:30 TU H2038

μSPD: A novel method for manufacturing of UFG wires and fibres — •Aikaterini Zi[1], Ralph Jörg Hellmig[1], Michael Kazakevich[2], Eugen Rabkin[2], and Juri Estrin[1] — [1]Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678 Clausthal-Zellerfeld — [2]Department of Materials Engineering, Technion, Haifa, Israel

Equal channel angular pressing (ECAP) is a well established technique for the production of ultrafine grained materials by severe plastic deformation. We propose a microscale analogue of ECAP. By using sub–millimeter sized channels in a process that is based both on the forcefill technology and severe plastic deformation concept, fibres or wires with ultrafine grain size could be manufactured. In these experiments porous filters with micrometer or submicrometer scale open porosity were used for the pressing of aluminium. First results demonstrate the viability of this approach, to which we refer to as μSPD. The technique can also be used for solid state infiltration of porous ceramic or metallic performs leading to fine grain size composites.

MM 25.5 Sa 15:45 TU H2038

Semi-Solid-Processing von X210CrW12 Werkzeugstahl: Simulation und Charakterisierung — •Dirk I. Uhlenhaut, Jürg Kradolfer, Jörg F. Löffler und Peter J. Uggowitzer — Laboratory of Metal Physics and Technology, ETH Zürich, Schweiz

Die Verarbeitung von Leichtmetalllegierungen im halbflüssigen Zustand erfreut sich zunehmender Bedeutung in Forschung und industrieller Anwendung. In der vorliegenden Arbeit wurde eine Werkzeugstahllegierung auf ihre Gefügeausbildung nach einer thermischen Behandlung im Erstarrungsintervall untersucht. Thermocalc-Simulationen wurden mittels optischer Mikroskopie, SEM und EDX verifiziert und die Eigenschaften der einzelnen Phasen im abgeschreckten Zustand sowie nach unterschiedlichen Wärmebehandlungen quantifiziert. Die Ausbildung und Stabilität der primären Austenit-Phase wurde simuliert und experimentell untersucht. Mikro- und Makrohärten, Verschleißwerte und Kerbschlagbiegeversuche nach verschiedenen Wärmebehandlungen bestätigten die Wettbewerbsfähigkeit des neuen Prozesses mit herkömmlicher Werkzeugstahlverarbeitung.

MM 25.6 Sa 16:00 TU H2038

Investigations on the rheological behaviour of semi-solid metallic alloys processed during Thixoforming — •Lars Pape, Michael Modigell und Markus Hufschmidt — Institut für Verfahrenstechnik der RWTH Aachen, Turmstr. 46, 52056 Aachen

Thixoforming is a shaping process situated between the conventional processes of casting and forging. The metallic alloy is processed as a metallic suspension (globular grains suspended in a liquid matrix), which is characterised by a complex flow behaviour.

This feature is analysed experimentally for Sn15Pb and A356 by performing specific rheological experiments in a Couette rheometer. The metallic suspensions show shear-thinning and time-dependent flow properties and exhibit a yield stress. The isostructural flow behaviour immediately after a change in shear rate indicates shear-thickening attributes. The flow behaviour is strongly influenced by the solid fraction, the particle shape and size and the degree of agglomeration of solid particles.

Based on the experimental results a mathematical model to describe the flow behaviour has been developed to use for numerical simulation of die filling processes. The modelling approach is based on a Herschel-Bulkley law to describe the shear-thinning properties and is extended by a structural parameter k to additionally consider the time-dependent properties of the material. After a change in shear rate, the structural parameter proceeds towards its equilibrium value corresponding to the actual shear rate. This transient variation is modelled by a first order rate equation where the rate constant changes whether a build-up or a destruction of the structure occurs.

MM 25.7 Sa 16:15 TU H2038

Oberflächenspannungen moderner Stahllegierungen — •Frank Schmidt-Hohagen, Jürgen Brillo und Ivan Egry — DLR - Deutsches Zentrum für Luft- und Raumfahrt / Institut für Raumsimulation / D-51170 Köln / Germany

Moderne Stahllegierungen sind in der Regel Mehrkomponentensysteme mit hochreaktiven, leicht flüchtigen Komponenten. Demzufolge erfordert deren Untersuchung in der flüssigen Phase extrem reine Prozess-Bedingungen. Diesem Umstand wurde bei der Konstruktion der verwendeten Elektromagnetischen Levitations-Anlage Rechnung getragen. Die Messung der Oberflächenspannungen erfolgte mit Hilfe der oscillating-drop-technique: bei dieser Methode werden Oberflächenschwingungen einer flüssigen, levitierten Metallprobe um ihre Gleichgewichtslage angeregt und kontaktlos mittels Hochgeschwindigkeitskamera detektiert. Die mit Hilfe von Fast-Fourier-Transformation (FFT) erzeugten Spektren liefern die Frequenzen der Oberflächenschwingungen und schließlich die Oberflächenspannung. Mit Hilfe dieser Methode wurden die Oberflächenspannungen industrieller Stahllegierungen im Rahmen des ESA Thermolab Projekts bestimmt. Diese Resultate werden vorgestellt und durch Vergleich mit Werten von reinem Eisen sowie binären und ternären Fe-Legierungen diskutiert.

MM 26 Hauptvortrag Cynthia Volkert

Zeit: Montag 09:45–10:15 Raum: TU H1058

Hauptvortrag MM 26.1 Mo 09:45 TU H1058

Size effects in metal plasticity — •Cynthia A. Volkert — Forschungszentrum Karlsruhe, Karlsruhe, Germany

Size effects in the plasticity of metal crystals are well known. In many metal samples decreasing the crystal volume leads to a strengthening effect. However some recent observations show that weakening may also occur, particularly in small crystals that are unconstrained by a substrate or surface oxide. These issues are very important in the assessment of the performance and reliability of metal features used in micro-systems and microelectronic devices, and even in nanostructured components. A summary of the apparent origins for size effects will be presented, including aspects of dislocation nucleation and motion, strain gradients, and sample surface conditions. The various contributions will be used to interpret recent results from uniaxial compression tests on micron-sized metal samples.

MM 27 Quasikristalle

Zeit: Montag 10:30–11:45 Raum: TU H111

MM 27.1 Mo 10:30 TU H111

Reversible Phase Transformation between amorphous and quasicrystalline state of ZrTiNiCu. — •S. Mechler, Ch. Abromeit, N. Wanderka, M.-P. Macht, G. Schumacher , B. Schattat, and S. Klaumuenzer — Hahn-Meitner Institut Berlin

During the crystallization process of several classes of metallic glasses quasicrystals are formed as the primary nucleating, intermediate phase. The alloy $Zr_{64.5}Ti_{11.4}Cu_{13.8}Ni_{10.3}$ can be produced by the splat quenching technique into amorphous sheets upto 50 μm thickness, whereas sheets of about 70-100 μm are fully quasicrystalline. Heating of the amorphous material leads at first to the transformation into the fully quasicrystalline state. The quasicrystals are metastable and vanish at higher temperatures in favor of crystalline phases. The phase transformations are investigated by means of DSC, XRD and TEM. To study the stability of quasicrystalline ZrTiCuNi under irradiation with swift heavy ions, we used Au, Xe and Kr ions in the energetic range of 300-600 MeV. Irradiation by 600 MeV Au, leads to full amorphization of the sample already for a fluence of 10^{13} /cm^2. At lower fluences, amorphous tracks inside the quasicrystals can be visualized by HRTEM. The amorphization of the quasicrystalline phase is ascribed to the high electronic energy loss of the Au ions (40 keV/nm). This state can be reversed again by heating.

MM 27.2 Mo 10:45 TU H111

Quasicrystal formation in mechanically alloyed Zr-Ti-Nb-Cu-Ni-Al glassy powders — •Sergio Scudino[1], Ludwig Schultz[1], Jürgen Eckert[2], Hergen Breitzke[3], and Klaus Lüders[3] — [1]IFW Dresden, Institut für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany — [2]FB 11 Material- und Geowissenschaften, FG Physikalische Metallkunde, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany — [3]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

Differently from the glassy $Zr_{57}Ti_8Nb_{2.5}Cu_{13.9}Ni_{11.1}Al_{7.5}$ melt-spun ribbon that forms an icosahedral quasicrystalline phase upon devitrification, the corresponding alloy produced by mechanical alloying of elemental powder mixtures does not clearly show quasicrystal formation. However, the addition of an appropriate amount of elemental zirconium to the mechanically alloyed powder changes the crystallization behavior inducing the formation of the quasicrystalline phase. This indicates that for this multi-component metallic glass quasicrystal formation in the mechanically alloyed powder is crucially linked to the composition rather than to the question whether there is a special quenched-in short-range order. This work was supported by the German Science Foundation under grants Ec 111/10-1,2 and Lu 217/17-1.

MM 27.3 Mo 11:00 TU H111

Multiscaling, Ergodicity and Localization in Quasiperiodic Chains — •V. Z. Cerovski[1], M. Schreiber[1], and U. Grimm[2] — [1]Institute für Physik, Technische Universität Chemnitz, D-09107 Chemnitz — [2]The Open University, Applied Mathematics Dept., Milton Keynes, MK76AA, UK.

We report results of numerical simulations of wavepacket dynamics in a class of chains consisting of two types of weakly coupled clusters arranged in a quasiperiodic sequence and investigate properties of eigenstates using the perturbation theory of degenerate levels in the coupling strength v and numerical diagonalization. Results show that wave packets anomalously diffuse *via* a two-step process of rapid and slow expansions, that persist for any $v > 0$. An elementary analysis of the perturbation theory of degenerate levels reveal that non-localized states appear only in sufficiently high order of perturbation theory that is simply related to the combinatorial properties of the sequences, and numerical diagonalization furthermore shows that eigenstates ergodically spread across the whole chain for $v > 0$, while in the limit $v \to 0$ ergodicity is broken and eigenstates spread only across clusters with the same number of atoms, in contradistinction with trivial localization at $v = 0$. Effects of the single-site perturbation on wavepacket dynamics are furthermore investigated and shown that by changing the position or strength of the impurity it is possible to control long-time wavepacket dynamics. By adding a single impurity it is possible to induce wavepacket localization on individual subchains as well as on the whole chain.

MM 27.4 Mo 11:15 TU H111

Electronic transport and structural properties of amorphous and quasicrystalline Al-TM thin films — •Jose Barzola-Quiquia and Peter Häussler — Institut für Physik, Technische Universität Chemnitz, D-09107, Germany

In the present contribution we present a detailed study and comparison of electronic transport properties and the atomic structure of the amorphous and the quasicrystalline state of Al(CuFe, PdMn, PdFe). The samples are prepared in situ at low temperature (T≈10K) as amorphous thin films. After preparation the samples were annealed at different temperatures and both, transport and structural properties were measured up to the transition to the quasicrystalline state at T>700K. The electronic transport properties show pronounced non- metallic behaviour versus temperature. The atomic structure is characterized by the typical spherical-periodic order of disordered systems. But, additional, local icosahedral order is observed, which gets more pronounced by annealing. This behaviours can be explained in the frame of an electronic stabilization of amorphous systems, very similar to Hume-Rothery alloys. Contrary to Hume-Rothery alloys, in the systems under consideration hybridisation effects between Al-$_p$ with TM-$_d$ electrons play an important rule. Our view on the electronic stabilization gets supported by electronic transport measurements.

MM 27.5 Mo 11:30 TU H111

Nichtkollineare magnetische Ordnung in Quasikristallen — •Elena Y. Vedmedenko[1], Uwe Grimm[2] und Roland Wiesendanger[1] — [1]Institut für Angewandte Physik, Jungiusstr. 11, 20355 Hamburg, Germany — [2]Applied Mathematics Department, The Open University, Milton Keynes MK7 6AA, UK

Die Grundzustandskonfigurationen eines Antiferromagneten, in dem die magnetischen Momente nach einer planaren quasiperiodische Parkettierung angeordnet sind, werden mittels Monte-Carlo Simulationen untersucht. Im Gegensatz zu der Situation für ferromagnetische Wechselwirkung [1] stellt sich heraus, dass das Zusammenspiel geometrischer Frustration und quasiperiodischer Ordnung zu einer dreidimensionalen nichtkollinearen antiferromagnetischen Struktur führt [2]. Diese besteht aus geordneten magnetischen Überstrukturen mit verschiedenen Energien und charakteristischen Wellenvektoren, in Abhängigkeit von der quasiperiodischen Anordnung der magnetischen Momente. Derartige Strukturen liefern eine mögliche Erklärung für die experimentell beobachteten kurzreichweitige magnetische Ordnung in ikosaedrischen Ho-Mg-Zn Quasikristallen [3].

[1] E. Y. Vedmedenko, H. P. Oepen and J. Kirschner, *Phys. Rev. Lett.* **90**, 137203 (2003).

[2] E. Y. Vedmedenko, U. Grimm and R. Wiesendanger, *Phys. Rev. Lett.* **93**, 076407 (2004).
[3] T. J. Sato, H. Takakura, A. P. Tsai, K. Shibata, K. Ohoyama and K. H. Andersen, *Phys. Rev. B* **61**, 476–486 (2000).

MM 28 Elektronische Eigenschaften

Zeit: Montag 10:30–12:00 Raum: TU H2038

MM 28.1 Mo 10:30 TU H2038

Surface Plasmon Resonance of Ag Nanotubes — •Yun Luo[1], Yixin Zhang[2], Martin Steinhart[1], Ralf B. Wehrspohn[3], Gunter Fischer[2] und Ulrich Gösele[1] — [1]Max-Planck-Institute of Microstructure Physics, Halle/Saale, Germany — [2]Max-Planck Research Unit for Enzymology of Protein Folding, Halle/Saale, Germamy — [3]Universität Paderborn, Warburger Strasse 100, Paderborn, Germany

Ag nanotubes and nanowires with outer diameters ranging from 25 nm to 400 nm and a shell thickness of 40 nm (in the case of tubes) have been fabricated via wetting of porous alumina templates and a subsequent annealing step at 350°C. Released nanotubes or nanowires with various diameters can be obtained by selectively removing the template.

In order to investigate the optical absorption properties of the 1D Ag nano-objects, they were dispersed in de-ionized water and placed in the beam path of a Hewlett-Packard Visible-ultraviolet spectrometer. During the measurement, the nanoobjects were kept suspended by stirring. The experimental absorption spectra carried out showed a sharp peak for Ag nanowires with a diameter of 25 nm at 374 nm. The peak position was shifted to longer wavelength and broadened when the diameter of the nanotubes was increasing.

FDTD calculations on both the transmission as well as the field distributions in the objects were performed assuming a dielectric constant corresponding to that of flat thin films. The calculated results show an agreement with the experiments curves

MM 28.2 Mo 10:45 TU H2038

Correlation-induced double-plasmon excitation in Al and Na — •C. Sternemann[1], S. Huotari[2], M. Volmer[1], G. Vanko[2], G. Monaco[2], M. Tolan[1], and W. Schülke[1] — [1]Institute of Physics, University of Dortmund, D-44221 Dortmund, Germany — [2]ESRF, BP 220, F-38043 Grenoble Cedex 9, France

Although the dynamic structure factor $S(\mathbf{q},\omega)$ of simple metals has been discussed extensively in terms of electron-ion interaction and electron-electron correlation, the separation of these two contributions in the analysis of $S(\mathbf{q},\omega)$ is not straightforward. In this study, a new type of structure in the $S(\mathbf{q},\omega)$ of simple metals was found. This structure originates solely from dynamic correlation effects in the homogeneous electron gas, and is not largely affected by electron-ion interaction.

The non-resonant inelastic x-ray scattering experiments have been performed at beamline ID16 of ESRF. The photon energy-loss spectra of both Al and Na have been measured for momentum-transfers between $0.7q_c$ and $1.5q_c$, i.e. across the plasmon cut-off vector q_c . For the first time, peaklike structures were found in the high-energy-loss tail of the dynamic structure factor of both metals. According to their shape, the q-dependence of their peak energies and intensities, these structures can be attributed to intrinsic plasmon-plasmon excitations, as proposed theoretically by Sturm and Gusarov [1]. Thus a new type of feature in S(q,w) has been observed which may give the opportunity to probe effects that are of second order in the dynamically screened Coulomb interaction.

[1] K. Sturm and A. Gusarov, Physical Review B **62**, 16474 (2000)

MM 28.3 Mo 11:00 TU H2038

Decoupling methods as dynamical mean field theory impurity solvers — •Harald Jeschke — Institut für theoretische Physik, Uni Frankfurt, Robert-Mayerstr. 8-10, 60054 Frankfurt/Main

The use of equation of motion decoupling methods as impurity solvers to be used in conjunction with the dynamical mean field self-consistency condition for the solution of lattice models is explored. By comparing the impurity solver to exact diagonalization results and applying it to lattice models like Hubbard model and Periodic Anderson model it is shown that the method could be a cheap alternative to computationally demanding methods like quantum Monte Carlo. The method works in a large range of parameters and promises to be useful in combination with density functional theory for the study of strongly correlated materials.

MM 28.4 Mo 11:15 TU H2038

Ab-initio Korrelationsrechnungen für V and Fe mit dem Lokalen Ansatz — •Gernot Stollhoff — Max Planck Institut f. Festkörperforschung, 70569 Stuttgart

Erstmals werden Resultate von ab-initio Korrelationsrechnungen mit dem Lokalen Ansatz für zwei Übergangsmetalle, nämlich V und (nichtmagnetisches) Fe präsentiert.

In beiden Fällen gibt es nennenswerte Abweichungen von den bekannten Dichtefunktionals (DF) - Resultaten. Bei V führen nicht lokale Austausch- und Korrelationsbeiträge zu einer Verschiebung der Fermiflächen und bringen sie in bessere Übereinstimmung mit dem Experiment. Bei Fe spielen diese Beiträge eine noch stärkere Rolle. Die Besetzungen in Hartree-Fock - und DF - Näherung unterscheiden sich gravierend. Die Besetzung des korrekten Grundzustandes liegt näher an der DF - Näherung, weicht aber deutlich ab. Entsprechend wird die Zustandsdichte modifiziert. Diese zeigt eine bessere Übereinstimmung mit den experimentellen Daten für Fe oberhalb des magnetischen Phasenüberganges.

MM 28.5 Mo 11:30 TU H2038

Al-TM(transition-metal) compounds: Non-isotropic electronic transport and bonding networks — •Torsten Schmidt and Heinrich Solbrig — Institute of Physics, Technical University of Chemnitz, D-09107

Alloys of these class, being similar to Si-based materials, cover a wide range of electronic properties between clearly metallic and even insulating. It has been shown experimentally[1] that covalent bonding is common in Al-TM systems.

A molecular-orbital analysis[2] reveals a strong bonding-antibonding splitting at next neighbors. We show that such bonds can combine to form extended bonding-networks which are covered by high valence density. Metallic systems of this kind have enhanced resistivities along directions which cross these bonding network.

We tread the above toppics in terms of a suitably defined network-bond-order by means of orbital based, as well as by scattering approaches.

[1] K. Kirihara *et al*. Phys. Rev. B68, 014205 (2003) [2] Krajčí and Hafner, J. Phys.: Condens. Matter 14, 5755 (2002)

MM 28.6 Mo 11:45 TU H2038

Redetermination and calculation of the thermopower of lead — •Horst Brodowsky and Matthias Albus — Institut f. Physikalische Chemie, Uni Kiel

Precise Thomson heat measurements by Roberts resulted in a shift of the previously accepted lead standard of Christian et al. by 0.30 μV/K. Superconductor measurements between 16 and 112 K suggest a shift of 0.41 ± 0.02 μV/K instead.

It has been shown for a number of transition metal alloys as well as for the alkali metals, that it is not necessary to calculate the ratio of the intractable transport coefficients of the Onsager equations. The diffusional thermopower happens to be equal to the more readily accessible entropy of the electrons divided by the electronic charge (Z. Metallkunde **90** (1999) 111; **91** (2000) 375; **93** (2002) 1164; **95** (2004) 698). This surprising result is obtained, because in metals the electron/atom ratio is constant along the length of the wire (besides the pressure) and the electrochemical potential of the electrons is a unique function of the temperature. This fact allows the more direct evaluation of Onsager's equation compared to the conventional method.

MM 29 Symposium Tomographic Methods in Materials Research Hauptvortrag Paul Midgley

Zeit: Montag 10:30–11:00 Raum: TU H1058

Hauptvortrag

MM 29.1 Mo 10:30 TU H1058

Nanoscale electron tomography for materials science — •P.A. Midgley, T.J.V. Yates, J.R. Tong, and I. Arslan — Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge, CB2 3QZ, UK

The explosion of interest in nanoscale structures and devices across a wide spectrum of materials brings with it a need for characterisation tools that will allow the structure, composition and other physical properties to be measured at the nanometre level and in three dimensions. Tomographic techniques enable the three-dimensional reconstruction of objects from a series of images, often recorded at successive tilts. Electron tomography in the transmission electron microscope has been used in various forms in the life sciences for over three decades to study many macromolecular structures, organelles, viruses and so on. However, it is only in the past five years that electron tomography has been used by those in the materials science community. In that short time it has changed from a technique of some curiosity to one which is now seen as a vital component in the armoury of any material microscopist. The rapid adoption of the technique has been driven in part by an automation of the electron microscope and a subsequent improvement in acquisition routines and by the introduction of new tomographic imaging methods that satisfy the projection requirement even for crystalline objects. In this paper I will present a number of examples of electron tomographic reconstructions, including carbon nanotubes, heterogeneous catalysts and intermetallic alloys that demonstrate how electron tomography can yield accurate, quantitative results at the nanoscale that cannot be achieved using any other technique.

MM 30 Symposium Tomographic Methods in Materials Research

Zeit: Montag 11:00–12:40 Raum: TU H1058

MM 30.1 Mo 11:00 TU H1058

Quantitative Field Determination for Magnetic Recording Heads — •Robert Ferrier[1] and Pat Ryan[2] — [1]Department of Physics and Astronomy, The University of Glasgow, Glasgow G12 8QQ, UK — [2]Advanced Transducer Development, Seagate Technology Inc., 7801 Computer Av. - M.S. NRW102, Bloomington MN 55435, USA

The magnetic recording industry is constantly striving to increase the areal density of information storage and currently 170Gbits/inch2 has been demonstrated. Track widths are now approaching 120nm and the high coercivity media employed require writing fields in excess of 0.4T and head flying heights of the order 20nm. Thus to assess the modelling of inductive head writing fields we must measure the field distribution at this distance or closer to the air bearing surface (ABS). The technique employed is electron beam tomography and the input data for the real space back projection method is obtained from orthogonal components of differential phase contrast image intensity obtained using a FEGSTEM instrument. The construction of the recording head combines the inductive writer in combination with a GMR reading head. The magnetic shielding poles for the latter are substantially longer than the width of the writing pole and if shadowing effects due to misalignment of the ABS in the microscope are to be minimised then only a small region (2.0x0.5μm2) around the writing polegap must remain in the original ABS plane. This is achieved by a combination of mechanical polishing, chemical etching and FIB milling. The determination of absolute field distributions for heads with writing pole widths 0.33μm and 0.22μm will be described and the future use of the method will be assessed.

MM 30.2 Mo 11:20 TU H1058

Electron Tomography for Materials Research and Indsutrial Applications — •Christian Kübel — FEI Company, Application Laboratory, Achtseweg Noord 5, 5651 GG Eindhoven, The Netherlands — Fraunhofer Institut für Fertigungstechnik und Materialforschung, Wiener Straße 12, 28359 Bremen, Germany

In recent years, the limitations of 'classical' electron microscopy in materials science characterization have become increasingly apparent. Especially in areas such as nanotechnology and the IC industry, accurate analysis and measurements for metrology are difficult to obtain as different features overlap in a single 2D projected (S)TEM image. Electron tomographic methods provide a way around these limitations and are capable of delivering nanometer resolution in 3D for relatively 'large' volumes. BF-TEM tomography techniques, traditionally used in life sciences, are only of limited use in materials science due to diffraction contrast. Therefore, we have developed an automated acquisition for HAADF-STEM tomography, which is easy to use for a wide range of (crystalline) materials. The possibilities of electron tomography for materials science will be demonstrated using catalyst, nanocrystal, and semiconductor materials. Important aspects of the tomography analysis will be determination of particle size distributions, analysis of morphologies and imaging of surface variations in 3D. Finally, the advantages and limitations of both BF-TEM and HAADF-STEM tomography for materials sciences will be discussed.

MM 30.3 Mo 11:40 TU H1058

Investigation of orientation gradients around particles and their influence on particle stimulated nucleation in a hot rolled Fe_3Al based alloy by applying 3D EBSD — •Joachim Konrad, Stefan Zaefferer, and Dierk Raabe — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str.1, 40237 Düsseldorf

The optimization of the mechanical properties of Fe_3Al based alloys requires the increase of room temperature ductility and of high temperature strength. Both can be achieved, inter alia, by the addition of particles, for example of Laves phase. On the one hand these particles influence recrystallisation by particle stimulated nucleation (PSN) or inhibition of boundary movement. On the other hand particles lead to strengthening of the matrix at high temperatures.

The occurrence of PSN is correlated with the size and the mechanical properties of the precipitates. The larger the particles are and the harder they are compared to the matrix the larger the orientation gradients in the matrix around these particles become. 3D EBSD investigations by serial sectioning using a scanning focused ion beam - electron microscope (FIB-SEM) reveal the spatial distribution of the orientation gradients and their influence on the nucleation behaviour. Furthermore, the orientation gradients provide information on the active slip systems in these areas.

MM 30.4 Mo 12:00 TU H1058

Electron Tomography of Nanoparticles: towards atomic resolution? — •Sara Bals[1], Christian Kisielowski[2], Mihail Croitoru[1], and Gustaaf Van Tendeloo[1] — [1]EMAT-University of Antwerp, Groenenborgerlaan 171, Antwerp B-2020, Belgium — [2]National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley CA 94720, USA

The use of bright field imaging for electron tomography in physical sciences is often hampered by the presence of Bragg diffraction. Reconstructions of Pt nanoparticles (5-7 nm) show that the morphology is not remarkably hampered, but artificial cavities are observed inside the particles. To understand the formation of these artifacts, we have used multislice calculations to simulate the different projections in a tomography series. From this we can conclude that strong scattering and channeling effects are possible reasons for the formation of the cavities. One of the experimental possibilities to overcome this problem is to combine electron tomography with annular dark field TEM. Here, the central beam and all electrons scattered up to a certain semi-angle are excluded from imaging by an annular objective aperture. In this manner, a mass-thickness contrast is generated that depends exponentially on sample thickness. Using this technique, we have successfully obtained a 3D reconstruction of CdTe tetrapods, which also allows us to locate the CdSe seed that is used during growth.

MM 30.5 Mo 12:20 TU H1058

Nanotomography with Scanning Probe Microscopy — •Robert Magerle — Institut für Physik, Technische Universität Chemnitz

Nanotomography [1] is a novel procedure for high-resolution volume imaging based on scanning probe microscopy (SPM). The method is similar to an excavation on the nanometer scale: With suitable etching of polishing techniques the specimen is eroded step by step and the chemical composition of each freshly exposed surface is imaged with scanning probe microscopy. From the resulting series of images, separated in depth by only a few nanometers, the specimen's three-dimensional microstructure can be reconstructed. I will present examples of volume images with 10 nm resolution of block copolymers, semi-crystalline polymers, and Ni-based superalloys; limitations and perspectives will also be addressed. With the success of SPM in mind, volume imaging with SPM promises new insights into the physics of materials on the nanometer and even atomic scale. [1] R. Magerle, Phys. Rev. Lett. 85, 2749 (2000); EP 1144989; U.S. Patent 6,546,788.

MM 31 Hauptvortrag Walter Wolf

Zeit: Montag 14:00–14:30 Raum: TU H1058

Hauptvortrag MM 31.1 Mo 14:00 TU H1058

Finite temperature ab initio modeling of formation and migration of impurities, point defects and planar faults — •Walter Wolf — Materials Design, Le Mans, France and Taos, (NM) USA

Ab initio methods have proved to be powerful in exploring properties of defects such as vacancies, antisites, impurities, stacking faults or grain boundaries. Nowadays, even temperature effects can be routinely included by ab initio lattice dynamics. In this contribution, emphasis is put on effects from finite temperature, defect migration and interaction.

Impurities are of large impact on phenomena such as stress corrosion cracking and may cause serious materials fatigue. Since cracking typically occurs at grain boundaries, a large variety of impurities (H, O, S, P, B, alloying metals) and combinations thereof are investigated for their impact on grain boundary cohesion in metals. Their statistic distribution is estimated from grain boundary and surface segregation energies and site preference energies. Temperature dependent energy and entropy contributions are included. As a result, candidates responsible for grain boundary weakening or strengthening are identified.

Formation and migration of point defects are studied. Energy profiles of diffusion paths are explored and metastable and transition states are analyzed thermodynamically. As a result, solubility and diffusion processes can be quantitatively predicted. In particular for hydrogen impurities, zero point vibrations are critically important. Taking into account temperature dependence enables reliable predictions at working temperature for technological applications, and has pushed the ab initio approach into direct application within the industrial research process.

MM 32 Poster TU B (Symposium Tomographic Methods in Materials Research M-32.32-55)

Zeit: Montag 14:30–16:30 Raum: Poster TU B

MM 32.1 Mo 14:30 Poster TU B

Surface morphology changes of 20 - 120 nm thin epitaxial Nb-films during hydrogen uptake — •Kai Nörthemann, Reiner Kirchheim, and Astrid Pundt — Institut für Materialphsysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The arrangement of phases in thin epitaxial films is presented in this contribution, using the model system Niobium-Hydrogen.

Because of the different lattice parameter of Niobium and Niobium hydride it is possible to study with the surface sensitive scanning tunneling microscopy (STM) the lateral arrangement of the α-phase and the hydride. STM pictures of thin epitaxial niobium films were taken during hydrogen loading, therefore the time dependency of the hydride formation can be examined. Different types of hydride arrangements were found. Their appearance will be discussed with regard to film thickness and roughness as well as substrate parameters. The stability of the arrangements will also be discussed.

This work is financially supported by the DFG via SFB 602.

MM 32.2 Mo 14:30 Poster TU B

Hydrogen sorption properties of Mg-1wt%Ni-0.2wt%Pd prepared by reactive milling — •O. Gutfleisch[1], S. dal Toe[1], M. Herrich[1], J. Zulkarnain[1], A. Handstein[1], and A. Pratt[2] — [1]IFW Dresden, Institut für Metallische Werkstoffe, Helmholtzstr. 20, D01069 Dresden, Germany — [2]Johnson Matthey Technology Centre, Reading RG4 9NH, UK

Despite the large differences in melting points and the high vapour pressure of Mg, we succeeded in the preparation of induction-melted Mg-1wt.%Ni-0.2wt%Pd alloy. The alloy was then reactively ball milled in 10 bar hydrogen. The structural changes during milling were characterised by XRD and high resolution scanning electron microscopy. The hydrogen sorption properties have been systematically studied by gravimetric analysis in a wide temperature and pressure range for absorption (1-10 bar, 50-300 °C) and desorption (250-350 °C, 50 mbar-1 bar). At 300 °C, the hydrogen absorption in 10 bar proceeds within less than 5 min reaching 6.3 wt% capacity; desorption in 50 mbar is completed within 10 min, whereas 20 min are needed when desorbing into 1 bar. Absorption conditions have been found to be very moderate: e.g. at 200 °C and 4 bar 5.5 wt.% is reached within 5 min, at 150 °C and 2 bar 5.0 wt.% is reached within 60 min and at 100 °C and 10 bar 4.0 wt.% is reached within 60 min. The combined effects of Pd and Ni additions prove particularly useful in providing superior kinetics at moderate charging conditions. Hydrogen capacity and kinetics did not deteriorate over at least 50 cycles. These data are compared with those of nanocrystalline MgH2 powders, obtained by intensive milling in argon atmosphere.

MM 32.3 Mo 14:30 Poster TU B

^{139}La-NMR and the metal-nonmetal transition of lanthanum hydrides — •Sandra Heck, Stephan Leyer, and Elmar Dormann — Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany

^{139}La Knight shift data [1] seemed in conflict with the disappearance of the conduction electron density of states deduced from specific heat measurements [2] for increasing hydrogen content in LaH_x ($2 \leq x \leq 3$) [3,4]. New data for Pauli susceptibility, ^{139} NMR line-width, line-shift and spin-lattice-relaxation are derived. Reliability of the $LaCl_3$ in aqueous solution Knight shift standard is questioned.

A conclusive picture based on NMR is presented.

Acknowledgment: R.G. Barnes and G. Majer for samples, DFG (Do 181/12) for financial support.

[1] R.G. Barnes et al, J. Less-Comm. Metals **1**72-174, 411 (1991)
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MM 32.4 Mo 14:30 Poster TU B

Herstellung und optische Eigenschaften von Seltenen-Erdhydriden — •H. Schröter und J. Schoenes — Institut für Halbleiterphysik und Optik, Mendelssohnstraße 3, 38106 Braunschweig

Seit längerem ist bekannt, dass Seltene Erdmetalle wie z.B. Yttrium, einen Metall-Isolator-Übergang zeigen, wenn sie einer Wasserstoffatmosphäre ausgesetzt werden. Die damit verbundene, Änderung der optischen Eigenschaften wurde mittels Ellipsometrie, u.a. am VUV-Ellipsometer am BESSY II, untersucht. Um den Mechanismus des Metall-Isolator-Übergangs zu verstehen, wurden Schichten mit unterschiedlicher Konzentration von Wasserstoff im Yttrium hergestellt und an ihnen Messungen durchgeführt. Zur Schichtherstellung wurden dabei verschiedene Methoden eingesetzt. Es wurden zum einem in-situ hydrierte Schichten mittles Molekularstrahlepitaxie (MBE) in einer Wasserstoffat-

mosphäre hergestellt, des weiteren wurde Schichten hergestellt, die nach dem Wachstum in einer an der MBE-Anlage angebrachten Wasserstoffzelle hydriert wurden. Zudem wurden noch Versuche unternommen, hydrierte Yttriumfilme durch Pulsed Laser Deposition (PLD) herzustellen.

MM 32.5 Mo 14:30 Poster TU B

Optische Untersuchungen an Selten-Erd-Hydriden im Bereich von 5meV bis 5eV — •S. Weber, D. Zur und J. Schoenes — Inst. für Halbleiterphysik und Optik, Mendelssohnstr. 3, 38106 Braunschweig

Viele Seltene-Erd-Metalle durchlaufen bei der Beladung mit Wasserstoff einen Metall-Isolator-Übergang. Neben den damit verbundenen dramatischen Veränderungen der elektrischen Eigenschaften werden die undurchsichtigen Metalle zu einem optisch transparenten Hydrid. Weiterhin geht bei Neodym und Europium eine Veränderung der magnetischen Eigenschaften zu ferromagnetischen Halbleitern einher.

Es wurden dünne epitaktische Filme aus Nd und Eu auf $CaF_2(111)$ und Si(111)-Substraten mittels Molekularstrahlepitaxie hergestellt. Auf CaF_2 wächst Nd im Lage für Lage Wachstum in hcp Struktur, während sich Eu im Stranski-Krastanov Wachstum in bcc Struktur abscheidet. Die Gitterfehlanpassung des Nd beträgt 5,2%. Augerelektronen-Spektroskopie Messungen belegen die chemische Sauberkeit der Filme. Die Transmission und Reflexion der Filme wurde im Energiebereich von 5meV bis 5eV gemessen, und der Metall-Isolator-Übergang anhand Messungen an Proben mit verschiedenen Wasserstoffkonzentrationen untersucht. Der Einfluß von Wasserstoffschwingungen ist im infraroten Spektralbereich anhand von Verschiebungen von Strukturen um den Faktor $\sqrt{2}$ zwischen hydrierten und deuterierten Eu-Filmen zu beobachten. Mit winkelaufgelöster Photoelektronenspektroskopie kann die Veränderung der elektronischen Zustandsdichte untersucht werden. Dazu wurden Messungen an metallischem und *in-situ* hydrierten Proben durchgeführt.

MM 32.6 Mo 14:30 Poster TU B

Mg-Ni-Y alloys as new negative electrode materials for Ni-MH rechargeable batteries — •Bogdan Khorkounov, Angelika Teresiak, Margitta Uhlemann, Annett Gebert, and Ludwig Schultz — IFW Dresden, Postfach 270116, 01171 Dresden

Mg_2Ni has a large theoretical discharge capacity, but slow hydrogen sorption kinetics and poor corrosion resistance. Microstructural refinement and further alloying are needed. Mg-Ni-Y alloys with amorphous/nanocrystalline structure are investigated regarding their hydrogenation behaviour and cyclic electrode performance. $Mg_{63-x}Ni_{30}Y_x$-alloys absorb electrochemically up to 2,2 wt. % [H]. The thermal behaviour of Mg-Y-Ni ribbons in the as quenched and hydrogen-charged state was studied by in situ XRD. Crystallisation starts at 423 K with formation of Mg_2(Ni,Y), metastabile Mg_6Ni, Mg. Samples with [H] < 0.6 wt. % show the same phase formation during heat treatment. The formation of Mg_6Ni is inhibited by increasing [H]. Mg_6Ni decomposes at $>$ 523 K into Mg, Mg_2Ni. [H] = 1.42 wt. % leads to the formation of the fcc complex compound Mg_2NiH_4 at 523 K under a hydrogen atmosphere of 0.5 MPa besides $Mg_2NiH_{0.2-0.3}$, YH_2, YH_3, MgH_2. Y improves the corrosion and cycle life stability of Mg_2Ni-based electrodes, but decreases the discharge capacity. The effects of alloy composition, microstructure and electrode preparation on the discharge characteristics are discussed.

MM 32.7 Mo 14:30 Poster TU B

Structure and Chemical Bonding in High Pressure Phases of the Heavy Pnictides, Sb and Bi — •Alim Ormeci and Helge Rosner — MPI CPfS Dresden, Germany

In recent years the high-pressure structures of Sb and Bi have been determined by very accurate experimental techniques. The sequence of the observed structural phase transitions are, in general, reproduced correctly by first-principles electronic structure methods. In this work we combine first-principles total-energy calculations with the topological analysis of the electron localization function (ELF) in order to study how crystal structure and bonding properties change as pressure is applied. Total-energy calculations are carried out by using the (i) full-potential linear muffin-tin-orbital method (FP-LMTO), and (ii) full-potential local orbital (FPLO) method. The ELF is calculated by using the FPLO method.

A particular issue is the importance of the relativistic effects to the electronic structure and to the crystal structure in Bi. This issue is investigated systematically by performing calculations based on the following approaches: (i) scalar relativistic Hamiltonian, (ii) spin-orbit coupling treated variationally, (iii) full Dirac Hamiltonian in a four-component implementation.

MM 32.8 Mo 14:30 Poster TU B

Electronic structure of Ga_{84} cluster compounds — •Johannes Frenzel, Sibylle Gemming, and Gotthard Seifert — Institut für Physikalische Chemie, TU Dresden, D-01062 Dresden

Semi-conducting and metal clusters as building blocks for organised structures are potential candidates for devices in nano electronics. In this field various aluminium and gallium clusters where synthesized with $[Al_{77}(N(SiMe_3)_2)_{20}]^{2-}$ and $[Ga_{84}(N(SiMe_3)_2)_{20}]^{4-}$ as the largest ones of this kind. Density functional calculations were carried out to study large bare and ligated gallium clusters and their packing in a three-dimensional crystal structure. In the single clusters, the electronic states are delocalised over the whole cluster and the gallium atoms exhibit no noticeable charge. Band structure calculations of the crystal do not yield any significant dispersion of the electronic bands. Thus it is concluded that the observed macroscopic electric conductivity is mediated by a hopping mechanism between the clusters rather than by the presence of states, which are delocalised over the whole crystal.

MM 32.9 Mo 14:30 Poster TU B

Diffusion und Viskosität in unterkühlten Metallschmelzen — •Alexander Bartsch[1], Klaus Rätzke[1], Volker Zöllmer[1], Andreas Meyer[2] und Franz Faupel[1] — [1]Technische Fakultät, Univ. Kiel, Kaiserstr. 2, 24143 Kiel — [2]TU München, Physik Department E13, James-Franck-Str., 85747 Garching

Seit der Entwicklung von Legierungen, die in der tief unterkühlten Schmelze stabil sind, werden Viskosität, Diffusion und Diffusionsmechanismus intensiv erforscht [1]. In der Gleichgewichtsschmelze gilt die Stokes Einstein Relation, nicht aber im Glaszustand. Daher bleibt offen, wo die Abweichung beginnt und welche Legierungskomponente die Viskosität bestimmt. An $Pd_{43}Cu_{27}Ni_{10}P_{20}$ wurden zwischen der kalorischen Glastemperatur $T_g = 582$ K und der kritischen Temperatur $T_c = 715$ K der Modenkopplungstheorie die Phosphor- und Cobalt-Diffusion gemessen. Der Vergleich von Co-Diffusion [2] und Viskosität [3] zeigt eine gute Übereinstimmung in der Gleichgewichtsschmelze. Mit fallender Temperatur beginnt ab T_c eine Divergenz von bis zu vier Größenordnungen bei T_g. Da die P-32-Diffusion in diesem Temperaturbereich fast so schnell wie Co-Diffusion ist, bestimmt erstere nicht die Viskosität; weitere Versuche mit Pd werden auf der Tagung präsentiert.

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MM 32.10 Mo 14:30 Poster TU B

Mechanical spectroscopy of Zr65Al7.5Cu27.5 thin films and first evidence for an excess-wing in metallic glasses — •Peter Rösner and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The double-paddle oscillator is used for the study of mechanical properties of thin amorphous Zr65Al7.5Cu27.5-films in the tempe-rature range from 300 to 650 K under ultra high vacuum conditions. The oscillator is driven in its secondary torsional eigenmode at about 5.4 kHz and the temperature dependence of the complex shear modulus of the film is measured. At temperatures above the glass transition, the loss modulus can be mathematically described by a Havriliak-Negami function. In the vicinity of the glass transition, our data clearly differ from this mathematical model. The temperature dependence of the mechanical loss modulus is very similar to the dielectric loss modulus of many other glass forming materials, where the deviation from the viscous alpha-process is described with an excess wing. Our experimental results give rise to the assumption that there exists a wing also in amorphous metals and could therefore be a universal property of glasses. One interpretation for the wing is to postulate density fluctuations and dynamic heterogeneities. Cooperative movement of groups of atoms that are called clusters and formed in the vicinity of the glass transition lead to a deviation of the alpha-process that is due to single-atom movement. The authors would like to thank P. Lunken-heimer and A. Loidl for many stimulating discussions. This work was supported by the Deutsche Forschungsgemeinschaft SFB 602, B8 and the Graduiertenkolleg 782.

MM 32.11 Mo 14:30 Poster TU B

DFT investigation of free and supported Mo_mS_n clusters — •Sibylle Gemming, Igor Popov, Jelena Tamuliene, and Gotthard Seifert — Institut für Physikalische Chemie, TU Dresden, D-01062 Dresden

The electronic and structural properties of clusters (Mo_nS_m) of the layered semiconductor MoS_2 were studied using density-functional based methods. For small Mo_nS_m clusters the evolution of structural elements, resembling the corresponding structure motifs of the layered bulk compound MoS_2 was found. Among the small clusters a highly symmetric Mo_4S_6 cluster features an outstandingly high stability and a large HOMO-LUMO gap. Thus, this cluster can be characterized as a "magic cluster". Mo_4S_6 forms stable, regular arrays on the Au(111) surface with a preferential adsorption of three sulphur atoms at Au-Au bridging positions. With increasing cluster size the stabilization of platelet structures is indicated. In the platelet structures the edges determine the deviation from the bulk properties. The binding energies increase smoothly with increasing cluster size towards the bulk limit. Small clusters and platelet structures have a HOMO-LUMO gap comparable with the gap of the semiconductor bulk material, whereas larger platelet structures show a metallic-like behaviour.

MM 32.12 Mo 14:30 Poster TU B

Phase-field model for binary alloys solidifying under stress — •Bo Liu and Klaus Kassner — Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg Postfach 4120, D-39016, Germany

A phase-field approach is developed to investigate the effect of compositionally-genarated elastic stresses on the morphological instability during directional solidification of a binary alloy. We present a detailed thermodynamic derivation of the model with antitrapping solute current in the mass convervation relation[A. Karma, Phys. Rev. Lett **87**, 115701 (2001)]. This antitrapping current counterbalances the physical, albeit artificially large, solute trapping effect generated when a mesoscopic interface thickness is used to simulate the interface evolution on experimental length and time scales. Furthermore, all spurious effects that scale with this thinkness can be suppressed after we introduce the different diffusivity of concentation evolution and elastic field evolution. The asymptotic analysis of the model recovers previous Gibbs-Thomson condition with compositionally-genarated elastic stresses [B.J. Spencer et.al, Acta metall. mater. **40**, 1599 (1992)]. The performance of the model is demonstrated by calculating accurately for the first time within a phase-field approach the oscillatory instability of a planar interface.

MM 32.13 Mo 14:30 Poster TU B

Strahlungsinduziertes Glätten innerer und äußerer Grenzflächen und Kornwachstum in Ni-Ag-Bilayern — •J. Petersen[1], K. Zhang[2] und S. G. Mayr[1] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, D-37073 Göttingen — [2]II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, D-37073 Göttingen

Es wurden Ni(45nm)-Ag(45nm)-Bilayer mit 300keV Xe^+-Ionen unterschiedlicher Fluenzen bestrahlt. Ionenbestrahlung bietet die Möglichkeit, innere und äußere Grenzflächen zu modifizieren und optimieren. Die wesentlichen morphologischen Änderungen in metallischen Systemen umfassen Glättung bzw. Aufrauung von Grenzflächen, sowie strahlungsinduziertes Kornwachstum. Neben Weitwinkel- und Kleinwinkelröntgenbeugungsmessungen wurde versucht, mittels Rastersondenmikroskopie und chemischen Ätzens direkt die Grenzfläche zu untersuchen. Das Ziel ist, die der Grenzflächenmodifikation zugrunde liegenden atomaren Mechanismen zu identifizieren. Eine wesentliche Rolle kommt hierbei dem thermal spike zu, der einerseits eine Strukturglättung durch viskoses Fließen hervorrufen kann, andererseits auch Rauigkeit und Ionenmischen induziert. Dieses Projekt wird im Rahmen des SFB 602 von der DFG gefördert.

MM 32.14 Mo 14:30 Poster TU B

Ferroic multilayers with highly mobile interface charges — •Sibylle Gemming and Gotthard Seifert — Institut für Physikalische Chemie, TU Dresden, D-01062 Dresden.

The multilayered system $SrTiO_3(001)|LaAlO_3(001)$ was investigated by density-functional band-structure calculations. For layers of equal and low thickness the optimised lattice constant equals the average of the ones of the two constituents. The system contains two different interface terminations with differing physical properties. For $SrO(001)|AlO_2$ (I) the interface spacing amounts to 1.90 Å, for $TiO_2(001)|LaO$ (II) the spacing is reduced to 1.86 Å. A model system with equal amounts of both terminations, is electronically neutral with an indirect band gap of about 2 eV and a direct one of 2.5 eV at the local-density level. Model systems with only termination I exhibit holes, localised in the O-based valence band; for systems with pure termination II the additional electrons occupy a Ti-based conduction band with stronger dispersion. Projections of the electron density show that both types of charge carrier are confined to the heterophase boundary region, and that the valence band holes are spatially more strongly localised than the additional conduction band electrons.

MM 32.15 Mo 14:30 Poster TU B

Curvature Driven Grain Boundary Motion in Aluminum. — •V.A. Ivanov[1], D.A. Molodov[1], L.S. Shvindlerman[1,2], and G. Gottstein[1] — [1]Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow Distr., 142432 Russia

The motion of individual grain boundaries under a constant driving force was studied in Al-bicrystals. In this technique the curved grain boundary moves along the lateral surface of the specimen forming a triple junction "free surface - boundary - free surface" during its motion.

Migration of different grain boundaries was measured *in-situ* utilizing orientation contrast in the SEM. The character of grain boundaries studied was described in terms of the crystallographic planes of the adjacent grains. In the current study, both effects the "surface" triple junction and the boundary character on steady state motion are considered. The effect of the junction is discussed with the criterion Λ which defines the influence of a triple junction on the motion of the attached grain boundaries. To describe the effect of boundary character, the shape of moving grain boundary was analyzed.

MM 32.16 Mo 14:30 Poster TU B

Dry sliding of copper tested by microtribometers in air and in vacuum — •Y. Liu, M. Gubisch, M. Himmerlich, S. Krischok, M. Scherge, and J.A. Schaefer — Institut für Physik und ZMN, TU Ilmenau, 98684 Ilmenau

At low speed and low load, mild wear was found in sliding tests of copper and its alloys. The mild wear is usually related to the formation of oxide films and influenced by the hardness of the substrates. If the oxide film remains after slider passes, and the substrate is hard enough to support the oxide film, the sliding occurs between the oxides, and thus a low wear and low coefficient of friction are expected. We examined this scenario by dry sliding tests of pure copper using microtribometers in air and in vacuum. The oxide films in the wear tracks were studied with scanning electron microscopy and photoelectron emission microscopy combined with locally resolved photoelectron spectroscopy. The deformation band underneath the wear tracks was revealed by conventional metallographic method and was observed by orientation imaging microscopy. The effect of the surface finishing and the atmospheric pressure on the coefficient of friction was examined, and discussed with reference to the formation of oxide films and the development of deformation band.

MM 32.17 Mo 14:30 Poster TU B

Defekte in extrem verformten CuZn-Legierungen - Experimente und Simulationen — •Kai Klement, Rolf Anders und Ferdinand Haider — Universität Augsburg

Durch das ECAP-Verfahren wird in den Proben eine hohe Zahl von Nichtgleichgewichtsdefekten wie Leerstellen und Versetzungen erzeugt. Das Ausheilen dieser Defekte wurde durch dilatometrische und thermoanalytische Methoden untersucht. Die Leerstellen haben einen größeren Anteil am Exzessvolumen, die Versetzungen liefern einen größeren Enthalpiebetrag. Bei diesen Messungen wurde je nach Zusammensetzung der CuZn-Proben (Cu mit bis zu 10 Gew.% Zn) eine Ausheilstufe zwischen 200°C und 300°C beobachtet. TEM-Aufnahmen sollen Aufschluss über die mikroskopischen Vorgänge geben.

Um den Beitrag der Versetzungen zur Volumenvergrößerung zu bestimmen, wurden außerdem Computersimulationen durchgeführt. Hierfür wurde ein fcc-Gitter mit zwei Stufenversetzungen erzeugt. Durch eine Relaxation mittels Molekulardynamik mit periodischen Randbedingungen und variabler Zellengröße wurde das mittlere Exzessvolumen der Versetzung bestimmt und mit einer entsprechenden Simulation ohne Versetzung verglichen. Darüberhinaus liefert die Konstruktion von Voronoi-Polyedern um die einzelnen Atome genauere Informationen über die Volumenvergrößerung in Abhängigkeit vom Abstand vom Versetzungskern.

MM 32.18 Mo 14:30 Poster TU B

Monte Carlo Simulation of Phase Separation Including Elastic Relaxations — •Rolf Anders[1], Gururajan Mogadalai Pandurangan[1,2], and Ferdinand Haider[1] — [1]Univ. Augsburg, Institut f. Physik — [2]Indian Institute of Science, Dept. f. Metallurgy

We developped a real space technique which includes local atomic relaxation during each atomic jump, allowing thus to study phase transformations with strong elastic contributions. For each atomic jump, the activation energy is computed using phenomenological interaction potentials. After a succesful jump the atomic coordinates of the vicinity of the jumping atom are relaxed in order to minimise the total energy. This method was applied to a Lennard-Jones alloy to study the microstructure evolution of two systems with respect to misfit parameter and temperature. In the first one the shape of the emerging precipitate phase was analysed, using a randomly mixed initial configuration. In the second one the changing shape of an initially spherical precipitate was investigated.

MM 32.19 Mo 14:30 Poster TU B

Novel conductor materials for high field pulsed magnets — •Alexander Gaganov, Jens Freudenberger, Ekaterina Botcharova, Elias Mohn, and Ludwig Schultz — Leibniz-Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, 01099 Dresden Germany

There is a need for high-strength and highly-conducting materials for applications such as pulsed high magnetic field coils. Three different approaches were studied in order to strengthen copper-based conductor materials. First, microcomposite Cu-Ag alloys yield high strength as a consequence of their nanoscale microstructure and, on the other hand, a Cu-based macrocomposite can be strengthened by the use of a steel jacket. Last, but not least Cu-Nb mechanically alloyed microcomposited bear large potential to be the futures material for this type of application. In all three cases the increase of strength coincides with a decrease of conductivity. Thus, the ideal material balances between these two competing properties. The actual results will be presented.

MM 32.20 Mo 14:30 Poster TU B

Molecular dynamics simulation of aluminium diffusion in decagonal quasicrystals — •Stephen Hocker and Franz Gähler — Universität Stuttgart, Institut für theoretische und angewandte Physik, 70550 Stuttgart

Aluminium diffusion in decagonal Al-Ni-Co and Al-Cu-Co quasicrystals is investigated by molecular dynamics simulations, using newly generated EAM potentials. As in our previous work with classical effective pair potentials, above two thirds of the melting temperature strong aluminium diffusion is observed. Compared to pair potentials, the diffusivities in the decagonal plane are enhanced, which is attributed to additional diffusion processes. Furthermore, with EAM potentials the transition metal atoms are more mobile, so that their diffusion is also measurable. The activation enthalpies and the activation volumes are determined by measuring the diffusivities as a function of temperature and pressure. The qualitative behavior of the dynamics is confirmed by ab-initio simulations.

MM 32.21 Mo 14:30 Poster TU B

Effective potentials from ab-initio data for decagonal Al-Ni-Co — •Peter Brommer and Franz Gähler — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Binary and ternary quasicrystalline alloys show remarkable mechanical and transport properties which one would like to reproduce and analyse in more detail in numerical experiments. Unfortunately, the required systems are several orders of magnitude too large for quantum mechanical methods. Classical molecular dynamics with effective potentials allow the simulation of much larger configurations, but for complex systems physically justifiable effective potentials are scarce. In the Force Matching method, data like forces, cohesive energies and stresses in small systems are calculated with ab-initio methods, and the parameters of an effective potential are adjusted to optimally reproduce these quantum mechanically determined data. In this work an effective potential for decagonal Al-Ni-Co obtained by Force Matching is presented and the application to other quasicrystalline systems is discussed.

MM 32.22 Mo 14:30 Poster TU B

Homogenous nucleation in supersaturated iron vapour, a molecular dynamics study — •Norbert Lümmen and Thomas Kraska — Universität zu Köln, Institut für Physikalische Chemie, Luxemburger Str. 116, D-50939 Köln

The nucleation rate is an important input parameter for the modelling of particle processes by continuum models such as population balances. With increasing nucleation rate more nuclei are formed in a given time range. The remaining atoms in the vapour phase are distributed over these particles over the course of the surface growth process. As result one obtains primary particles which are smaller than in case of a lower nucleation rate.

The experimental investigation of the nucleation at extreme conditions such as high temperature or high pressure is often difficult. In this work we show how molecular dynamics simulations can be employed for the investigation of the homogeneous nucleation and the calculation of nucleation rates for such systems. It is also shown how the obtained nucleation rate can be compared with available experimental data.

MM 32.23 Mo 14:30 Poster TU B

New Expression for the Diffusivity of Carbon in Fe-C Austenite — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt

In engineering technology of particularly case or through hardenable low-alloyed steels, precise mathematical prediction and analysis of carbon solid-state diffusion profiles is of special importance to proper heat treatment process control (carburization) and failure inspection (decarburization). Thus, reliable input data is required for correct simulations. Evaluating three discrete literature sources, for the concentration dependence of the carbon diffusivity in austenite linearized representations suitable for computing-time saving iterative calculations are derived between 0 and 1.4 m.% C and fitted with respect to temperature in the practically most relevant range form 1073 to 1373 K by means of two equivalent defining equations based on a simple polynomial expression and a physically founded Arrhenius approach, respectively. An extensive comparison to available literature references, which are partly inconsistent with each other, is drawn. The mathematical analysis of an industrial two-step gas carburizing experiment demonstrates the potential of the new expression.

MM 32.24 Mo 14:30 Poster TU B

New Computer Model for Decarburization of Steels with Simultaneous Carbide Dissolution — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt

Decarburization, i.e. outward diffusion of carbon caused by oxidation reactions, seriously impairs the mechanical edge zone properties of the affected material. This process represents the most important undesirable side effect to common heat treatment (e.g. austenitizing, soft annealing) and hot-working operations (e.g. forging, upsetting) of particularly low-alloyed steels. Reliable simulation tools are thus required for substantiated failure analyses. If the initial carbon content of the steel exceeds its solubility in austenite, decarburization is accompanied by carbide dissolution and thus becomes a complex diffusion process with simultaneous chemical reaction. A realistic computer model for the involvement of this background process, based on an iterative solution of Fick's law, is developed. Applying the novel calculation tool, the effect of the rate constant of carbide dissolution on the carbon profiles is discussed in detail considering decarburization of standard rolling bearing steel 100Cr6 (SAE 52100) in contaminated protective atmosphere under usual austenitizing conditions at 1123 K as example.

MM 32.25 Mo 14:30 Poster TU B

Thermo-physical properties of thin film and FIB modified NiTi shape memory alloys — •Jürgen Gibkes[1], Ch. Zamponie[2], R. Wernhardt[3], B.K. Bein[1], and J. Pelzl[1] — [1]Solid State Spectroscopy, Experimantal Physics 3, Ruhr-University, D-44780 Bochum — [2]Cesar Research Center, D-53175 Bonn — [3]Experimental Physics 6, Ruhr-University, D-44780 Bochum

Thermal transport parameters are key parameters for the functionality of shape memory (SM) material. The need of miniaturisation of the SM devices requires alternative preparation techniques of the base material affecting the thermal transport parameter. We have investigated films of a few microns thickness and bulk samples laterally surface modified by FIB (focus ion beam). The NiTi films were prepared by sputtering. After removing the amorphous films from the substrate they are thermal

treated in order to induce a crystalline structure. The thermal transport properties were investigated by frequency dependent photothermal infrared radiometry. The annealed films exhibit different thermal parameters as the bulk materials of the same composition. The FIP prepared samples were investigated with a scanning thermal microscope (SThM). Local changes of the thermal transport properties with different doses were measured with a resolution of about 50 nm.

This work was performed in the frame of the Sonderforschungsbereich 459.

MM 32.26 Mo 14:30 Poster TU B

Microstructure, phase sequence, and superelasticity in highly oriented MBE-grown NiTiCu shape memory thin films — •R. Hassdorf[1], J. Feydt[1], S. Thienhaus[1], M. Boese[2], L. Buforn[3], N. Conté[3], and M. Moske[1] — [1]Forschungszentrum caesar, 53175 Bonn, Germany — [2]Universität Bonn, Institut für Anorganische Chemie, 53117 Bonn, Germany — [3]CSM Instruments SA, 2034 Peseux, Switzerland

Using MBE deposition highly oriented NiTiCu shape memory thin films were accomplished. The austenite-martensite transition in these films, single or two-stage transformation depending on the quantity of the Cu additions, occurs with comparable transition temperatures as known for sputter-deposited films. Mechanical stress measurements reveal a deformation recovery in the order of 400 MPa. Superelasticity spans to about 3% strain as referred to spherical indentation data. The microstructure is remarkable in that the crystallites are oriented within $\pm 5^\circ$ along the film plane normal as observed by X-ray diffraction. The occurrence of this preferential order is deduced to the formation of a Ti-rich (Ti_2Ni) phase at the film-substrate interface providing a highly oriented initial crystallization template. The results described in this study outline the perspectives for tailoring the microstructure and transformation performance of shape memory thin films, especially in regard to technological applications.

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MM 32.27 Mo 14:30 Poster TU B

Fluid Flow Effects on Phase Formation and Microstructural Evolution in Nd-Fe-B Melts — •Sven Reutzel[1,2], Takeshi Okutani[3], Thomas Volkmann[2], Jianrong Gao[4], Jörn Strohmenger[2], Heinrich Bach[1], and Dieter M. Herlach[2] — [1]Ruhr-University, Bochum — [2]German Aerospace Center, Cologne — [3]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan — [4]Northeastern University, Shenyang, China

Experiments on peritectic and hyper-peritectic $Nd_xFe_{100-1.5x}B_{0.5x}$ alloy melts (x = 11.8, 14, 16 and 18) were performed under microgravity during parabolic flight campaigns using the TEMPUS facility (Tiegelfreies elektromagnetische Positionieren unter Schwerelosigkeit) to elucidate the effect of melt convection on critical undercooling levels for the occurrence of metastable phases and the different solidification pathways which were observed in ground-based electromagnetic levitation experiments. Furthermore, the experiments were carried out to improve the knowledge on the relationship between undercooling, fluid flow, magnetic field, metastable phase formation and the structural properties, such as the homogeneity and crystallite orientation. Our main focus was (I) to analyse the influence of fluid flow in the undercooled melt on phase selection and on volume fraction of competing phases in the solidified samples and (II) to evaluate the influence of convection and static magnetic fields with respect to the crystallographic alignment of grains and homogeneity of microstructure.

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MM 32.28 Mo 14:30 Poster TU B

Hochtemperaturkorrosion von Überhitzerrohren in Kraftwerken — •Barbara Waldmann[1], Bernhard Stöcker[1], Christoph Mocker[1], Ferdinand Haider[1], Siegfried Horn[1] und Ragnar Warnecke[2] — [1]Institut f. Physik, Univ. Augsburg — [2]GKS Gemeinschaftskraftwerk, Schweinfurt

Die Korrosion von Stählen in Wärmetauschern von Kraftwerken ist nach wie vor nicht in allen Einzelheiten verstanden. Insbesondere in Müllverbrennungsanlagen ist die Korrosion ein erhebliches technisches und auch wirtschaftliches Problem. Am Beispiel eines häufig eingesetzten niedrig legierten Kohlenstoffstahls (15Mo3) wurde in einem Modellexperiment der Korrosionsangriff in einer chloridhaltigen Atmosphäre bei ca. 400°C (der typischen Arbeitstemperatur) mittels Rasterelektronenmikroskopie und EDX untersucht. Daneben werden Korrosionsstrom und -spannung mit elektrochemischen Methoden registriert. Es zeigt sich, dass sich auf dem Stahl zunächst eine Eisenchloridphase bildet, oberhalb derer als stabiles Korrosionsprodukt Eisenoxide wachsen. Diese Ergebnisse stimmen qualitativ mit den Befunden an aus einer MVA entnommennen Stahlproben überein.

MM 32.29 Mo 14:30 Poster TU B

Molekulardynamik-Simulationen zum Skalenverhalten der Schmelztemperatur von metallischen Nanopartikeln — •Magnus Kreth und Peter Entel — Universität Duisburg-Essen, Institut für Physik, 47048 Duisburg

Das Schmelzen von metallischen Nanopartikeln wurde mit Hilfe von Molekulardynamik-Simulationen untersucht. Wir studieren das Skalenverhalten der Schmelztemperatur für eine Reihe von metallischen Systemen. Die interatomaren Wechselwirkungen in den Simulationen werden durch empirische tight-binding second moment Potentiale beschrieben.

MM 32.30 Mo 14:30 Poster TU B

Microstructure of Fe2Re (Re=Tb, Nd) spherical alloy produced by containerless solidification in drop tube — •Shumpei Ozawa[1,2], Kazuhiko Kuribayashi[1], and Dieter Herlach[2] — [1]Institute of Space and Astronautical Science, 3-1-1 Yoshinodai, Sagamihara, 229-8510, JAPAN — [2]Institute of Space Simulation, German Aerospace Center, 51170 Cologne, GERMANY

Fe2TbxNd1-x alloy were containerlessly solidified in a drop tube. Droplets of various diameters were formed and collected at the bottom of the drop tube. The microstructures of the Fe2Tb samples consist of two regions. One is properitectic Fe3Re phase in the Fe2Tb matrix and the other is primary Fe2Tb dendritic grains. The region that consists of Fe2Tb dendrite expands due to the enhancement of the undercooling and cooling rate with decreasing the sample diameter. In the Fe2Tb0.5Nd0.5 samples, the Fe3Re phase crystallized from the melt directly. The Fe2Re phase is peritectically formed from Fe3Tb and liquid phases. The further improvement in the solidification conditions such as the ejection gas pressure and temperature of the molten metals together with the composition modifications should be favorable to increase the undercooling level for the direct crystallization of the Fe2Re phase. This will be a challenge to produce the Fe2Nd Laves phase directly from the undercooled melt, which has been theoretically predicted to exhibit the highest magnetostrictive strain.

MM 32.31 Mo 14:30 Poster TU B

Martensitic transformation behavior of compression aged Ni-rich NiTi shape memory alloys — •J. Michutta[1], Ch. Somsen[1], A. Dlouhy[2], K. Neuking[1], and G. Eggeler[1] — [1]Institute of Materials Science, Ruhr-University Bochum, 44780 Germany — [2]Institute of Physics of Materials, Zizkova 22, 61662 Brno, Czech Republic

In the present study we investigate the martensitic transformation behavior in Ni-Ti single crystals with a nomin al Ni content of 50.8at.% aged under compression of 50MPa in [111]-direction for aging times from 2ks up to 360ks at 550°C. The martensitic transformation behavior of the compression aged single crystals is mainly characterize d by differential scanning calorimetry (DSC) and in-situ transmission electron microscopy (TEM) on cooling the sa mples. Compression aging at 550°C in [111]-direction leads for all investigated aging times to the growth of only one family of Ni_4Ti_3 precipitates. In order to reduce internal stresses the Ni_4Ti_3 precipitates grow in an autoc atalytic process resulting in B2-type channels in between the precipitates. On cooling three peaks are present in the DSC charts, more distinct for the longer aging times from 16ks up to 360ks. In-situ TEM shows that the first peak on cooling is attributed to a martensitic transformation of the high temperature B2-phase to the martensiti c R-phase starting at the particle matrix interface all over the sample. In contrast the second peak is associate d with the formation of B19′ in favorite regions of the single crystal appearing in a burst like event on cooling in some channels. On further cooling from this transformed channels the martensitic B19′-phase growth, which exp lains the third peak in the DSC-measurements.

MM 32.32 Mo 14:30 Poster TU B

NON-DESTRUCTIVE TESTING WITH NEUTRON PHASE CONTRAST IMAGING — •Klaus Lorenz[1], Erich Steichele[1], and Eberhard Lehmann[2] — [1]FRM-II, 85748 Garching, Germany — [2]Paul-Scherrer-Institut, 5232 Villigen, Switzerland

At the NEUTRA facility (SINQ), a great variety of objects was investigated with phase contrast radiography, for instance metal foams and

casted objects. The phase contrast effect is now well understood and great efforts are made to improve the existing setup and to exploit all the possibilities offered by this technique. The tomography facility ANTARES at the FRM-II in Garching was designed to perform phase contrast measurements with neutrons as a matter of routine.

A big goal is to do quantitative phase contrast radiography and the step towards phase contrast tomography. By performing phase retrieval for every slice of a tomographic data set it becomes possible to assign every voxel the imaginary (attenuation coefficient) and the real part of the refractive index. This allows the separation of materials, which could not be separated hitherto in conventional tomographies.

MM 32.33 Mo 14:30 Poster TU B

Conceptual design and construction of the cold neutron tomography facility at HMI — •André Hilger[1,2], Nikolay Kardjilov[1], Lounis Mokrani[1], Rudolf Ringel[1], Wolfgang Treimer[1,2], and John Banhart[1] — [1]Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin — [2]Technische Fachhochschule Berlin, Luxemburger Str. 10, 13353 Berlin

Neutron tomography is a powerful non-destructive method for the investigation of a large variety of different objects. It allows to visualize the inner volume of a sample without destroying or dismantling it. The different interaction mechanisms of neutrons and X-rays with matter make neutron tomography a complementary technique to classical X-ray tomography. Tomographic imaging with cold neutrons is on one hand highly sensitive to light elements and organic materials. On the other hand, cold neutrons pass easily through metals and other materials composed of heavy elements. A new tomography facility with cold neutrons is under construction at the reactor BER II of the Hahn-Meitner-Institut, Berlin. The new instrument is placed at the end of a curved neutron guide which faces the cold neutron source of the reactor. Two measuring positions are planned. The first one is directly at the end of the neutron guide where an extremely high cold neutron flux of approximately $10^9 n/cm^2 s$ is available. The second measuring position is intended for high-resolution tomography and is located 5 m away from the neutron guide where the flux is only $10^7 n/cm^2 s$ but the beam collimation is much better. The first test experiments at these measuring position have been performed and will be presented.

MM 32.34 Mo 14:30 Poster TU B

Tomography with Monochromatic Neutrons — •Markus Strobl[1,2], Wolfgang Treimer[1,2], André Hilger[1,2], and Nikolay Kardjilov[1] — [1]Hahn-Meitner-Institut Berlin, Glienickerstr. 100 14109 Berlin — [2]Technische Fachhochschule Berlin, Luxemburger Str. 10, 13353 Berlin

A perfect Si monochromator placed in the cold neutron beam of the BER II reactor at the Hahn-Meitner-Institute provides a highly monochromatic beam. The ratio $\Delta\lambda/\lambda$ is in the range of a few percent for a wavelength $\lambda = 0.45nm$ that is fulfilling the Bragg condition for the asymmetric reflection. Although the resulting flux density is low i.e. approximately $5 \times 10^3 cm^{-2} s^{-1}$ this beam has advantages for special radiography and tomography applications. On one hand the effect of beam hardening can be avoided and hence a better sensitivity concerning slight density differences can be achieved. On the other hand the irradiation of samples can be reduced compared to high flux instruments in spite of the fact that the exposure time is necessarily increased. The spatial resolution of the instrument can be given with $125\mu m$ in horizontal respectively $200\mu m$ in vertical direction. Some examples of successful applications will be given.

MM 32.35 Mo 14:30 Poster TU B

Combination of neutron tomography and X-ray tomography at FRM-II — •Michael Schulz and Burkhard Schillinger — Technische Universität München, 85747 Garching, Germany

The combination of neutron tomography and x-ray tomography can greatly enhance the field of application of computed tomography in non-destructive testing. Having different absorption coefficients for x-rays and neutrons, respectively more materials can be distinguished than with only one of the two methods. One of the major problems of combining different imaging methods is the alignment of the 3D datasets to each other (image registration). This difficulty can almost completely be avoided by using the same measuring geometry and detector setup for both measurements. For neutron tomography the radiographies are made in parallel beam geometry. As a detector we use a neutron sensitive scintillation screen and a CCD camera to record the scintillation image. Increasing the distance between our 320kV x-ray source and the sample position to approx. 12m, a nearly parallel beam geometry can be achieved for x-ray tomography, either. Thus it is possible to use the same reconstruction algorithm for the two datasets. This minimizes the differences in shape and orientation of the two 3D datasets. The detector is the same CCD camera as for neutron tomography in combination with a scintillation screen which is sensitive to both x-ray and neutrons. In this talk we will present the new x-ray tomography facility at the experimental reactor FRM-II in Garching. First experimental results will be shown and our experience with the new facility will be discussed.

MM 32.36 Mo 14:30 Poster TU B

Einfluss auf die Relaxationraten T_1 und T_2 durch Kombination von NMR und NAR — •David Tyler Hartman, André Engelbertz und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms- Universität zu Bonn

NMR ist heutzutage ein vielfältig eingesetztes Werkzeug in der naturwissenschaftlichen Forschung bis hin zum Klinikalltag. Durch die physikalisch begründeten Relaxationszeiten ist diese Methode für Betrachtungen von dynamischen Prozessen in der Bildgebung bisher ungeeignet. An Festkörpern kann auf die Relaxationszeiten mit Hilfe von eingestrahltem und resonantem Ultraschall Einfluss genommen werden. Desweiteren werden Messungen an weicher Materie und Flüssigkeiten vorgestellt. Dafür wurde der Ultraschall mit der Lamorfrequenz unter dem optimalen Winkel von 54,7° eingestrahlt. Die Ultraschallpulse erzeugen über periodische Druckschwankungen Wechselfelder, vergleichbar zum B_1-Feld, welche mit dem Kernspinensemble wechselwirken. Die Resultate an den verschiedenen Proben werden hier vorgestellt.

MM 32.37 Mo 14:30 Poster TU B

Nonlinear registration of series of atomic force microscopy images of nanostructured materials — •Sabine Scherdel[1], Stefan Wirtz[2], Nicolaus Rehse[1] und Robert Magerle[1] — [1]Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth — [2]Mathematisches Institut, Universität zu Lübeck, 23560 Lübeck

Nanotomography is a new method to map the complex spatial structure of modern materials. Here a series of two-dimensional atomic force microscopy images is obtained. To reassemble these to a volume image image distortions must be corrected. We have modified a more general registration method [1] for our applications, which was mainly applied to medical science so far. Our atomic force microscopy images are cutouts of an object and show not a single object that is clearly separated from the background. Furthermore the selected section is slightly shifted in each image. Inevitable contaminations of the specimen are another problem. They appear in just one layer and contribute with high grey values to the calculation of the distortion field, even though they comprise no three-dimensional image info rmation at all. By the use of this nonlinear registration we are able to picture nanostructured materials over large ranges (1 mum) with a resolution of 10 nm per pixel. Examples are a 20 nm wide rack in a nickel based super alloy as well as several crystalline lamellae in a semi-crystalline polymer film.

[1] B. Fischer, J. Modersitzki, J. of Math. Imag. Vision 2003, 18, 81.

MM 32.38 Mo 14:30 Poster TU B

Tomographic atom probe (TAP) study of the chemical ordering in amorphous alloys — •Ahmed Shariq, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich hund platz 1,D 37077, Göttingen, Germany

Amorphous alloys are characterized by the absence of atomic long range order and reveal only topological and sometimes chemical short range order. The attractive properties offered by these alloys triggered intensive microstructural investigations in the last few years. The wider supercooled liquid region in new amorphous alloys allows to explore the kinetics and thermodynamics in this region. Atomic scale chemical ordering in such alloys put great demands on the characterizing techniques. The 3D-tomographic atom probe (TAP) is proved to be currently the best experimental tool to gain information on chemical heterogeneities at the atomic scale. The data from TAP has been used to elucidate the atomic distance between neighbouring atoms. The chemical ordering in the Fe, Pd and Zr based amorphous alloys are discussed in this contribution.

MM 32.39 Mo 14:30 Poster TU B

Analysis of Ordering and Site Occupancies in TiAlNb — •Torben Boll[1], Talaat Al-Kassab[1] und 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, Nanjing 210093, China

Titanium-aluminium-alloys with small amounts of Niobium were prepared under high vacuum conditions by means of levitation melting. Heat treatment in the temperature range of 1250 K for several hours were performed.

The samples were investigated with field ion microscopy (FIM) and tomographic atom probe (TAP). Special attention was paid to the distribution of Nb in the γ-phase, where it, as FIM-analysis indicates, preferentially occupies Ti-sites. A new algorithmic approach based on TAP-data was developed to evaluate the site occupancies in ordered structures. Preliminary results, obtained with this method, will be presented and discussed for the site occupancy of Nb along a <001>-direction in these alloys.

MM 32.40 Mo 14:30 Poster TU B

New aspects of the decomposition in CuCo observed with different field ionisation-based tomographic techniques — •Alexander Heinrich, Talaat Al-Kassab und Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

CuCo has been of great interest as an ideal model system for decomposition in binary alloys. Specimen of Cu2at.%Co have been examined using the Tomographic Atom Probe (TAP), Field Ion Microscopy (FIM) and a recently developed method for Field Ion Image Tomography (FIIT). In this method sequences of field evaporation images are digitally registered. A three dimensional reconstruction of the imaged volume is followed via an advanced algorithm. This enables the examination of large analysis volumes with respect to the volume analysed in the TAP. New aspects of the decomposition behaviour at lower annealing temperatures (703K and 763K) could be observed with this technique. Nucleation is observed initially along the elastic soft direction in Cu, forming needle-shaped precipitates which are subsequently subject to coarsening reactions. In contrast to this phase separation at higher annealing temperatures (853K) was observed to take a different path of decomposition. Small agglomerates of atoms form which then coarsen to larger precipitates. The results will be discussed in terms of phase decomposition theory.

MM 32.41 Mo 14:30 Poster TU B

Segregation and Clustering of Phosphorus at Grain Bounderies of Nanocrystalline Cobalt — •Catharina Wille[1], Taláat Al-Kassab[1], Reiner Kirchheim[1], Melina da Silva[2], and Uta Klement[2] — [1]Georg-August-Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37075 Göttingen — [2]Chalmers University of Technology, Department of Material Science and Engeneering, SE-412 96 Göteborg, Schweden

Nanocrystalline Co-1.2at%P and Co-2.1at%P layers with a thickness of 70-200 μm and a grain size of around 10 nm were prepared by pulsed current electrodeposition. These specimens were investigated by Field Ion Microscopy (FIM), Tomographic Atom Probe (TAP) and Transmission Electron Microscopy (TEM) both in the as prepared state and after different heat treatments.

The results reveal already a P-segregation at the grain boundaries in the as prepared state. In addition to normal and abnormal grain growth, the Co-1.2at%P alloy exhibited the formation of Co_2P- and CoP-precipitates at grain boundaries after isochronal thermal annealing. In this paper, preliminary results of grain growth and segregation behavior as a function of temperature and time of annealing for the Co-2.1at%P alloy will be presented. The findings will be compared to the ones observed in the Co-1.2at%P alloy.

MM 32.42 Mo 14:30 Poster TU B

Analysis of the ageing of metallic foams by means of quantitative micro-computed tomography (μCT) — •Oliver Brunke[1], Stefan Odenbach[1], and Felix Beckmann[2] — [1]ZARM Universität Bremen, Am Fallturm, 28359 Bremen — [2]GKSS-Forschungszentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht

Metallic foams, and especially those made from Al and its alloys, have become a major topic for both industrial and basic research throughout the last decade. The physical properties of solid metallic foam which are relevant for most applications like e.g. in automotive or aerospace industry are strongly affected by its structure parameters, like for instance pore size, shape and distribution, the location of inhomogeneities or the distribution of solid material between films and Plateau borders. On the other hand, these parameters directly depend on the temporal development, stability and ageing of the liquid foam system. The ageing behaviour of Al foams produced by a powder metallurgical route has been observed by means of Synchrotron- as well as cone beam μCT. We will present methods for the analysis of the development of the structure of metallic foams using 3D image processing techniques. This allows us the three dimensional and non-destructive determination of the temporal behaviour of e.g. the pore size or the cell wall material of the foam system.

MM 32.43 Mo 14:30 Poster TU B

High resolution synchrotron tomography on Nickelbase superalloys — •Thomas Link[1] und Alexander Epishin[2] — [1]Dr. T. Link, TU Berlin BH18, Ernst-Reuter-Platz 1, 10587 Berlin — [2]Dr. A. Epishin, BAM-Berlin, Unter den Eichen 87, 12205 Berlin

Single crystals of Nickel base superalloys contain micro pores, resulting from solidification, heat treatment and creep deformation. The investigated specimens have rod shape. They are grown by directional solidification, resulting in a dendritic structure along the rod axis. SEM images of cross sections through the rods gave an indication, that the pores are arranged preferably in the interdendritic region. Because the pore volume fraction is quite low, about 0.3 percent, this is difficult to be seen in a 2D image. Therefore tomography was applied. The pores under interest are quite small, around 5 microns, and the density of the superalloys high. This restricted the thickness of the specimens to about 0.5mm. They were investigated at the ID19 beamline, ESRF, Grenoble under 50 keV. The main points of interest were: Porosity in undeformed superalloys of the 3 generation (SRR99, CMSX-4, CMSX-10). Development of porosity in CMSX-4 during creep. Influence of the creep stress on the creep porosity. We could show, that porosity is most pronounced in the newest superalloy. Porosity increases during creep. With rising creep stress the creep pores form also in the primary and secondary dendrite arms.

MM 32.44 Mo 14:30 Poster TU B

Development and construction of an X-ray nano-tomography facility for interdisciplinary research at the Ghent University — •Bert Masschaele[1], Manuel Dierick[2], Jelle Vlassenbroeck[2], Luc Van Hoorebeke[2], Patric Jacobs[1], and Veerle Cnudde[1] — [1]Krijgslaan 281, S8, B-9000 Gent — [2]Proeftuinstraat 86 B-9000 Gent Belgium

Development and construction of an X-ray nano-tomography facility for interdisciplinary research at the Ghent University

Bert Masschaele b, Manuel Dierick a, Jelle Vlassenbroeck a , Luc Van Hoorebeke a, Patric Jacobs b, Veerle Cnudde b

a Proeftuinstraat 86 B-9000 Gent b Krijgslaan 281, S8, B-9000 Gent

Since very recent is has become possible to manufacture X-ray tubes with high energy and high flux with focal spot sizes below 1 micrometer. These sources make it possible to investigate samples with a resolution below 1 micrometer and a detail detectability of 200nm non-destructively and in three dimensions. In the paper we will discuss the development of a nano-tomograph for multidisciplinary research. We will also discuss the latest evolutions of the detectors and manipulation motors for sub micrometer tomography.

MM 32.45 Mo 14:30 Poster TU B

Server/Client Distributed Cone Beam Reconstruction algorithm — •Jelle Vlassenbroeck, Bert Masschaele, Manuel Dierick, and Luc Van Hoorebeke — Proeftuinstraat 86 B-9000 Gent Belgium

Server/Client Distributed Cone Beam Reconstruction algorithm

Jelle Vlassenbroeck, Bert Masschaele, Manuel Dierick, Luc Van Hoorebeke

Ghent University Proeftuinstraat 86 B-9000 Gent

During the last 10 years micro-CT has gained much popularity in industry and research. A lot of efford was put into the development of fast reconstruction algorithms and dedicated hardware to improve the CT reconstruction calculations in terms of speed and quality. In the past year we have developed a dedicated FDK algorithm using LabVIEW for the Octopus package. The paper will explain the new algorithm and the server/client implementation for network reconstruction.

MM 32.46 Mo 14:30 Poster TU B

Chemical processes in commercial batteries studied by synchrotron-tomography and 3D image analysis — •A. Rack[1], A. Haibel[1], I. Manke[2], S. Zabler[2], H. Riesemeier[3], G. Weidemann[3], J. Goebbels[3], and J. Banhart[1,2] — [1]Hahn-Meitner-Institut Berlin, Abteilung Strukturforschung, Glienicker Str. 100, 14109 Berlin — [2]Institut für Metallphysik, Hardenbergstr. 36, 10623 Berlin — [3]Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, Haus 60, 12205 Berlin

Batteries are playing a major role in everybody's daylife: laser pointers, walkmen, mobile telephones - all are working with a power pack. Here we are focusing on manganese-zinc batteries (type AAA/micro) as they are widely used and therefore investigations are interesting for all kind of applications. By working with the high resolution tomographic setup of the BAMline @ BESSY II we obtained 3D images of one battery in different discharging stages. Due to the use of monochromatic radiation we are able to distinguish between the different materials within our tomographic image. All chemical components are separated from the greyscaled data into Boolean images and then evaluated by 3D image analysis methods derived from stochastic geometry [1]. We can quantify the time-dependent decay of the battery's manganese as well as changes of the zinc powder's morphological structure.

[1] J. Ohser and F. Mücklich, *Statistical Analysis of Microstructures in Materials Science*, John Wiley & Sons, 2000

MM 32.47 Mo 14:30 Poster TU B

Study of semi-solid casting and processing with X-ray phase-sensit ive tomography — •S. Zabler[1], A. Haibel[2], A. Rack[2], A. Rueda[1], H. Riesemeier[3], G. Weidemann[3], J. Goebbels[3], and J. Banhart[1,2] — [1]Institut für Werkstoffe (TU), 10623 Berlin — [2]Hahn-Meitner-Institut Berlin, Abteilung SF3, 14109 Berlin — [3]Bundesanstalt für Materialforschung und -prüfung, 12205 B erlin

Alloys with a *globular microstructure* are the feedstock for industr ial components processed in the *semi-solid state* which requires thi xotropic behaviour of the melt. The fundamental link between alloy micros tructure and *thixotropic breakdown*, occuring when shear stress is a pplied, was first reported for Sn-Pb15 (Spencer 1972). During the past th ree decades thixo-processing has been established for a wide range of all oys but structural analysis remained however limited to metallography (2D images) and rheology (global measurement of viscosity as a function of s hear rate, temperature and shear time). Non-destructive three-dimensional structure analysis was first performed at the ESRF in 2000. It initiated a new rush for the investigation and modelling of the semi-solid casting process. In a first approach we use alloys with higher absorption contra st than common Al-Si in order to characterize the three-dimensional image s of *dendritic* and *globular* structures. Then we show recent e xperiments from the tomography setup of *BAMline* at the synchrotron BESSYII. The setup provides high spatial resolution using X rays with a *partial spatial coherence* thus allowing 3D *phase-sensitive imag ing* of neighbouring elements that are undistinguishable to absorption to mography.

MM 32.48 Mo 14:30 Poster TU B

High resolution synchrotron-tomography on human tooth tissue — •H. G. Gräber[1], A. Rack[2], A. Haibel[2], I. Manke[3], H. Riesemeier[4], G. Weidemann[4], J. Goebbels[4], and J. Banhart[2,3] — [1]Medical Faculty, RWTH Aachen — [2]Hahn-Meitner-Institut Berlin, Abteilung Strukturforschung — [3]Institut für Metallphysik, TU Berlin — [4]Bundesanstalt für Materialforschung und -prüfung

Caries and periodontitis are the most frequent infectious diseases at all. Both diseases lead to an irreversible loss of mineralized tissues (bone and tooth). The aim of current and future research projects is to develop regenerative strategies by means of tissue engineering. We examine samples for different stages of the disease with synchrotron-tomography using a high spatial resolution of 1.5 μm pixelsize. The demineralized tissue can be detected in the 3d images due to it's lower density. By quantitative analysis of the data one obtains information about the disease growing's time-dependence. A comparison of non-treated infected teeth with treated ones (e.g. fluoridation) delivers information about the quality of different regeneration approaches.

MM 32.49 Mo 14:30 Poster TU B

Flaw Types in Metallic samples Analyzed with Computed Tomography — •Juergen Goebbels, Gerd Weidemann, Heinrich Riesemeier, Bernhard Illerhaus, and Yener Onel — BAM, Unter den Eichen 87, 12205 Berlin

Volume characterization of metallic samples with computed tomography requires a broad spectrum of X-ray energies depending on the maximum material thickness to be penetrated. BAM has developed several tomographs from high resolution computed tomography with synchrotron radiation at the BAMline at BESSY in the energy range from 8 to 80 keV, over laboratory equipment using different kind of microfocus X-ray tubes (a 100 kV transmission type X-ray tube, a conventional 225 kV and a world wide unique 320 kV bi-polar microfocus X-ray tube) up to high energy sources like Co-60 and an 12 MeV electron linear accelerator. The limits of spatial and contrast resolution are discussed together with the types of detectors used. The flaw types ranges from different kind of pores and cracks in welding seams to stress corrosion cracking, inclusions and inhomogenities.

MM 32.50 Mo 14:30 Poster TU B

3D reconstruction of an abnormally growing Goss grain in Fe3%Si by FIB serial sectioning and EBSD — •Dorothée Dorner and Stefan Zaefferer — Max-Planck-Institut für Eisenforschung, Abteilung Mikrostrukturphysik und Umformtechnik, 40237 Düsseldorf, Germany

Grain-oriented silicon steel is used in electrical transformers as the core material. It is characterised by a strong crystallographic preferred orientation that develops due to abnormal (discontinuous) growth of {110}<001>-oriented grains (Goss grains). Though various models exist to explain this abnormal growth behaviour, no theory is yet generally accepted. The $\Sigma 9$ grain boundary theory emphasis the significance of special grain boundaries. The solid state wetting model is based on grain boundary energy considerations and proposes a special grain boundary shape, i.e. wedge-shaped bulges.

In this study, we performed serial sectioning experiments with the focussed ion beam (FIB) technique in combination with crystal orientation measurements using electron backscatter diffraction (EBSD). We investigated the shape of growing Goss grains in 3D as well as the spatial position and crystallography of their grain boundaries. This possibly helps to answer how the anisotropic growth of Goss grains depends on the grain boundary properties.

MM 32.51 Mo 14:30 Poster TU B

3D-analysis of the crystal orientation relationship and growth process of lenticular martensite in Fe-30mass%Ni alloy — •Hisashi Sato and Stefan Zaefferer — Department of Microstructure Physics and Metal Forming, Max-Planck-Institute for Iron Research, Max-Planck-Strasse, 1, Dusseldorf, Germany

The 3-dimensional structure of lenticular martensite in Fe-Ni alloys has been studied by EBSD orientation microscopy on serial sections produced in a focused ion beam - scanning electron microscope (FIB-SEM). With a spatial resolution of 50 x 50 x 50 nm and an orientation resolution of 0.5° very fine details of the microstructure can be observed and a formation mechanism is proposed.

In previous studies [1-2], it has been reported that the crystal orientation relationship (OR) between martensite and austenite in Fe-Ni alloy is Nishiyama-Wassermann. However, this OR is an average one which can only partly be confirmed by our local measurements. The 3-dimensional measurements show that martensite nucleates with a Kurdjumov-Sachs relationship which then rotates towards NW with further growth.

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1. W.P.Liu and H.J.Bunge: Mater. Lett.,10(1991)343.
2. G.Bruckner, A.Kontges and G.Gottstein: Steel Res.,70(1999)188.

MM 32.52 Mo 14:30 Poster TU B

Investigation of rheological behaviour of binary alloys with synchrotron radiation — •Rueda A.[1], Zabler S.[1], Rack A.[2], Haibel A.[2], and Banhart J.[1,2] — [1]Technische Universität Berlin, Institut für Werkstoffwissenschaften und -technologien, Fakultät III - Fachgebiet Struktur und Eigenschaften von Materialien — [2]Hahn-Meitner-Institut Berlin, SF3, Abteilung Werkstoffe

Thixotropic alloys are characterized by a non-dendritic, i. e. globular, solid phase embedded in a melting liquid matrix. Due to the good casting property of the thixotropic alloys they play an important role for engineering applications. One production route of such alloys is the new

rheocasting process. At this, the liquid alloy will be casted in a special container and the accruing shear forces cause the building of the globular solid structure. By using this proceeding and with chemical grain refining (AlTiB) we were able to manufacture thixotropic material (AlGe15%) with around 100μm diameter grains. In order to investigate the static and dynamic, i.e. rheological, properties we used synchrotron radiation at BESSY II. By means of high resolution synchrotron radiography we studied the microstructure of our alloy, which is rich in absorption contrast of X-rays. Tomographic images of the thixotropic alloy are used to quantify their globular shape. In radiographic images of micrometer-thin layers we obtained at real time the rheological behaviour, i.e. the grain formation and movement in the mushy state of the alloy.

MM 32.53 Mo 14:30 Poster TU B

Synchrotron Tomography Investigations on Ceramic Foams — •A. Berthold[1], A. Haibel[2], and H. Schubert[1] — [1]TU Berlin, Institut für Werkstoffwissenschaften und -technologien, Fakultät III - Fachgebiet Keramik — [2]Hahn-Meitner-Institut Berlin, SF3 Abteilung Werkstoffe

Interfacial active properties of special biopolymers, i.e. proteins, allow the generation of ceramic foams with microwaves. This differs obviously from conventional production methods of such foams. By means of synchrotron tomography we investigated the mechanism of accruement of the initial pore distribution in these foams as well as the shape of fully foamed ceramic material. Thanks to the knowledge of the accruement mechanism we are able to influence and control pore accruement and growth.

MM 32.54 Mo 14:30 Poster TU B

Ausbau der Mikrotomographieapparatur für Serienuntersuchungen von Magnesiumimplantaten — •J. Fischer[1,2], F. Witte[1], T. Donath[2] und F. Beckmann[2] — [1]Orthopädische Klinik der Medizinischen Hochschule Hannover, Anna-von-Borries-Str. 1-7, 30625 Hannover — [2]GKSS Forschungszentrum, Max-Planck-Str. 1, 21502 Geesthacht

Die Mikrotomographie mit Synchrotronstrahlung ist in der Materialwissenschaft zu einer festen Größe geworden. Am Deutschen Elektronen-Synchrotron DESY werden unter Verwendung der Tomographieapparatur der GKSS unter anderem Untersuchungen von Magnesiumimplantaten der Medizinischen Hochschule Hannover durchgeführt. Um Serienuntersuchungen zu beschleunigen, wurden ein automatisches Probenwechselsystem, sowie der Umbau auf eine kontinuierlich drehende Rotationsachse realisiert. Es wird das Konzept und die Durchführung der Umbauten dargestellt.

MM 33 Symposium Tomographic Methods in Materials Research
Hauptvortrag Cloetens

Zeit: Montag 16:30–17:00 Raum: TU H1058

Hauptvortrag MM 33.1 Mo 16:30 TU H1058

New trends in synchrotron-based tomography — •Cloetens P. — ESRF, F-38043 Grenoble Cedex

MM 34 Symposium Tomographic Methods in Materials Research

Zeit: Montag 17:00–18:00 Raum: TU H1058

MM 34.1 Mo 17:00 TU H1058

Application of discrete tomography to multi-level images and real projection data — •Zoltán Kiss[1], Attila Kuba[1], Antal Nagy[1], and Márton Balaskó[2] — [1]Dept. of Image Processing and Computer Graphics, University of Szeged, Hungary, H-6701 Szeged, Hungary, P. O. Box 652. — [2]KFKI Atomic Energy Research Institute, H-1525 Budapest 114, Hungary, P.O. Box 49.

Discrete tomography is an imaging technique to reconstruct discrete images from their projections using the knowledge that the object to be reconstructed contains only a few homogeneous materials characterized by known discrete absorption values. By this assumption the reconstruction can be done from relatively few projections and efficiently used in industrial non-destructive material examination. In previous research a stochastic reconstruction technique was successfully applied to binary phantom images, which considers the reconstruction as an optimization task. Now an extension of this method is introduced, which reconstructs multi-level phantom images from a few noisy projections and additionally we discuss the effect of several reconstruction parameters. We provide our experiments based on real measured projections including the possible improvements, reduction of the noise effect, building in a priori information, and a comparison with the classical FBP reconstruction method.

MM 34.2 Mo 17:20 TU H1058

Asymmetric Bragg Reflection As Magnifying X-Ray Optics — •Peter Modregger, Peter Schäfer, Daniel Lübbert, and Rolf Köhler — HU - Institut für Physik

Generally, the resolution limit for x-ray images is determined by available detectors (few 10μm). The x-ray image magnification with asymmetric Bragg reflection is a promising way to overcome this resolution limit, simultaneously providing a high detector efficiency and a strong phase contrast. However, the imaging process is currently not understood in detail. With a theoretical description of the imaging process and numerical simulations we have shown that the resolution limit is in the sub-micrometer regime for pure absorption objects and that it even improves for the more realistic case of phase objects. In the latter case, it turns out that the resolution limit depends on the phase object itself. This technique of x-ray imaging can be combined with tomographic reconstruction and we have demonstrated the practicability using an object with almost absent absorption contrast.

MM 34.3 Mo 17:40 TU H1058

3-D X-ray imaging: Current status and future developments at HGHG-FELs — •Gerd Schneider — BESSY m.b.H., Albert-Einstein-Str. 15, 12489 Berlin

The full-field x-ray microscope installed at the 3rd generation electron storage ring BESSY II is dedicated for applications in life, environmental and materials sciences. It covers the photon energy range between 250 - 750 eV. Currently, the spatial resolution is about 20 nm. Due to the small numerical aperture of zone plates, X-ray objectives have a depth of focus on the order of several microns. By treating the X-ray microscopy images as projections of the sample absorption, computed tomography can be performed.

3-D x-ray microscopy - pioneered at the BESSY I electron storage ring - has found numerous applications worldwide. To further improve 3-D x-ray imaging towards 10 nm spatial resolution and to increase the usable photon energy range into the hard x-ray region, progress has to be made in nanotechnology of the x-ray optics, the instrumentation and the theory for recovering the full 3-D information of an object at this resolution level. In the talk, the current status at synchrotron sources and future aspects of x-ray imaging with fs-pulses from Free Electron Lasers will be discussed.

MM 35 Hauptvortrag Karl Maier

Zeit: Dienstag 09:45–10:15 Raum: TU H1058

Hauptvortrag MM 35.1 Di 09:45 TU H1058

Prediction of material fatigue — •Karl Maier — Helmholtz Institut für Strahlen und Kernphysik, Nußallee 14-16, 53115 Bonn

About 30 years ago positron annihilation became a useful tool in basic metal research eg. vacancy formation enthalpies of nearly all metals could be measured with high precision in thermal equilibrium. In the meantime the experimental techniques and the theoretical understanding developed to a high standard. Position resolved measurements with a resolution of a few microns are now possible in a standard laboratory.

The consequent next step is to take laboratory techniques and knowledge into an industrial environment. There are many relevant material problems which can be solved with positron annihilation. Without any sample preparation, plastic zones in front of fatigue cracks are visible in a non-destructive way. First precursors of material failure at extremely low concentrations can be used to estimate the fracture within only 1% of cycles in a Wöhler experiment. Examples in light alloys, ferritic and austenitic steels are discussed.

MM 36 Symposium Tomographic Methods in Materials Research Hauptvortrag Astrid Haibel

Zeit: Dienstag 10:30–11:00 Raum: TU H1058

Hauptvortrag MM 36.1 Di 10:30 TU H1058

Synchrotron X-ray microtomography: principles and applications — •A. Haibel, A. Rack, S. Zabler, and J. Banhart — Hahn-Meitner-Institut Berlin, Abteilung Strukturforschung, Glienicker Str. 100, 14109 Berlin

Synchrotron tomography images the interior structure of real objects three-dimensionally, non-destructively, and with a high spatial resolution. This allows for a detailed microstructural analysis of many different kinds of materials or small engineering components. The wide field of applications of synchrotron microtomography will be presented by means of several examples, i.e. metallic foams, thixotropic alloys as well as further components and materials. Our research topics aim at the understanding of the structural and chemical nature of these objects. Moreover, by in-situ experiments, reorganization processes, e.g. the discharge process inside an alkaline battery or the accumulation of SiC particles on the pore surfaces in metallic foams during the foaming process will be visualized and characterized quantitatively. All presented results were measured at the tomographic facility of the BAMline at the BESSY II synchrotron.

MM 37 Symposium Tomographic Methods in Materials Research

Zeit: Dienstag 11:00–12:40 Raum: TU H1058

MM 37.1 Di 11:00 TU H1058

3D-Atom Probe investigation of carbide dissolution in a pearlitic steel subjected to severe plastic deformation. — •Yu. Ivanisenko[1], X. Sauvage[2], H. Rösner[1], and H.-J. Fecht[1,3] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [2]Institut des Matériaux de Rouen, Université de Rouen, BP 12, 76801 Saint-Etienne-du-Rouvray, France — [3]Abt. Werkstoffe der Elektrotechnik, Universität Ulm, 89081 Ulm, Germany

Pearlitic steels find a wide application in industry mainly as a material for rails and tyre cords. Phenomenon of decomposition of carbides occurring either during the exploitation of rails, or during the cold drawing of wires is very important because it decreases the ductility, and consequently leads to the loss of mechanical properties.

The application of 3D Atom Probe to study the process of strain induced cementite dissolution in pearlitic steels is very promising because it allows to detect the concentration of the elements in alloys with atomic resolution. Here we report our results on 3D AP investigation of pearlitic steel (Fe - 0.76 wt. % C - 1.2 wt. % Mn) following the room temperature severe plastic deformation by high pressure torsion. We show that decomposition of carbides starts already in the beginning of straining with a gradual decrease of the carbon concentration and formation of transitional non-stoichiometric phases with carbon contents of 8-16 at. %. A parallel HRTEM investigation has demonstrated that these phases, still keeping the lamellar shape, are partially amorphous. Increasing the strain further leads to a considerable decrease of size and amount of such carbon-rich areas and formation of carbon segregations on grain boundaries of nanocrystalline ferrite and along the dislocations.

MM 37.2 Di 11:20 TU H1058

Stability and Thermal Reaction of GMR NiFe/Cu Thin Films — •Constantin Buzau Ene[1], Guido Schmitz[2], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen — [2]Institut für Materialphysik, Wilhelm-Klemm-Str. 10, D-48149 Münster

Giant magneto-resistance (GMR) model systems of NiFe/Cu multilayer stacks with 2 nm single layer thickness were deposited onto needle-shaped W tips using ion beam sputtering and analyzed by atom probe tomography (TAP) after appropriate heat treatments.

Owing to the outstanding sensitivity of the method, even minor chemical modifications on the nanometer scale can be detected. Although annealing treatments at temperatures up to 250°C result already in a dramatic decrease of magneto-resistivity, no major structural or chemical transformation of the initial layer system is found. Instead, a slight decrease of the concentration slope at the interfaces is observed, which is attributed to short range interdiffusion induced by non-equilibrium point defects. Annealing at higher temperatures up to 500°C/40 min still preserves a clear layer structure. However, appreciable amounts of Ni are dissolved inside the Cu layers. In presence of grain boundaries, the onset of significant grain boundary diffusion is at about 350°C.

According to the nanoanalysis, the low temperature breakdown of the magneto-resistivity in NiFe/Cu systems is related to the short range interdiffusion of Ni in Cu on a mixing width of about 1nm, which happens homogeneously along the interfaces without destroying the clear layer structure.

MM 37.3 Di 11:40 TU H1058

Tomographic characterization of magnetic sensor materials — •Guido Schmitz[1], Constantin Ene[2], and Mario Kuduz[2] — [1]Institut für Materialphysik, Westf. Wilhelms-Univ., Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institut für Materialphysik, Univ. Göttingen, Friedrich-Hundt-Platz 1, 37077 Göttingen, Germany

Atomprobe tomography provides a 3D local chemical analysis with atomic sensitivity. Due to the 3D chemical information, atomic transport processes can be determined even in complex nanocrystalline materials. The application of the method to thin film multilayers is demonstrated at the example of magneto resistive sensor devices. Investigations of {NiFe/Cu/Co/Cu}, {Cu/Py}, {Co/Al_2O_3/NiFe} systems are presented. These structure are severely unstable from a thermodynamic point of view, so that their thermal stability and reaction gets an important issue for any technical application. Based on the 3D volume reconstruction, different mechanisms of atomic transport are identified and their relative importance for the degeneration of the giant magneto resistance effect or the electrical stability of tunnel barriers determined. According to the nano-analysis, volume diffusion induced by non-equilibrium point defects seems to be the dominant factor in GMR systems. In oxide tunnel barriers, a thermal treatment leads to zones of local enrichment of metallic impurities, which probably induces electrical breakthroughs.

MM 37.4 Di 12:00 TU H1058

Characterization of precipitates in aluminum based alloy AW 6016 — •N. Wanderka, R. Schiffmann, and J. Banhart — Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany

The aluminium based engineering alloy AW 6016 of nominal composition 98.44 Al - 0.45 Mg - 0.96 Si - 0.11 Fe - 0.034 Mn - 0.0054 Zn - 0.0038 Cr (at. %) was investigated. Heat treatment of solutionized and quenched alloys leads to an increase in hardness which is due to the formation of small precipitates of nanometer size. Two complementary high resolution methods, namely transmission electron microscopy (TEM) and three - dimensional atom probe (3 DAP), are used for investigations of the precipitate evolution after annealing at 185°C and 235°C. At very early stages, i.e. after 5 min at 185°C, Mg-rich, Si-rich and Mg-Si co-clusters are observed. They are spherical and their diameter is between 1 and 3 nm. The number density of clusters as measured by 3 DAP is 9 x $10^{23}/m^3$. After ageing for 25 min and 90 min at 185°C GP zones needle-shaped β" phases are formed. Both are rich in Mg and Si. The concentration ratio of Mg to Si of the precipitates is approximately 1. The number density of all precipitates after 90 min annealing time at 185°C is 6 x $10^{23}/m^3$. The needle-like β" precipitates at this ageing stage are about 4 nm in diameter and longer than 10 nm. The precipitates formed at 235°C after 10 min are much larger compared to those at 185°C. They are rod-shaped and have an average size as measured by TEM, about 50 nm in length and 3-4 nm in cross-section. The concentration ratio between Mg and Si as measured by 3 DAP is about 1.

MM 37.5 Di 12:20 TU H1058

Untersuchung des Materialflusses beim Reibrührschweißen mit Synchrotronstrahlung basierter Mikrotomographie — T. Donath, F. Beckmann, R. Zettler, A. Schreyer, •T. Donath, F. Beckmann, R. Zettler und A. Schreyer — GKSS Forschungszentrum, Max-Planck-Str. 1, 21502 Geesthacht, Deutschland

Die Außenstelle des GKSS Forschungszentrums bei DESY, HASYLAB betreibt eine Apparatur für röntgenmikrotomographische Untersuchungen an der Synchronstrahlungsquelle DORIS.

Es wurden in Reibrührtechnik hergestellte Schweißnähte einer Aluminiumlegierung mit Hilfe dieser Apparatur untersucht. Der bei dieser Schweißtechnik auftretende plastische Materialfluss konnte durch das Einbringen von Ti-Pulver in den tomographischen Rekonstruktionen sichtbar gemacht werden. Die Mikrotomographie-Apparatur und die Untersuchungsergebnisse werden vorgestellt.

MM 38 Mechanische Eigenschaften I

Zeit: Dienstag 10:30–11:30 Raum: TU H111

MM 38.1 Di 10:30 TU H111

Zerstörungsfreie Lebensdauervorhersage dynamisch beanspruchter Bauteile — •Ingo Müller[1], Karsten Bennewitz[2], Matz Haaks[1], Andreas Puls[1], Christiane Zamponi[1], Torsten E. M. Staab[1] und Karl Maier[1] — [1]Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn, Nußallee 14-16, D-53115 Bonn, Germany — [2]Zentrallabor Volkswagen AG, 38436 Wolfsburg

Für die Lebensdauervorhersage von dynamisch beanspruchten Bauteilen ist die Kenntnis eines Wöhlerdiagramms notwendig. Die Erstellung eines Wöhlerfeldes ist jedoch insbesondere für große Lastzyklenzahlen ($>10^7$ Zyklen) sehr zeitaufwendig. Mit der Positronenannihilationspektroskopie kann die Entstehung der Fehlstellen in der Probe zerstörungsfrei verfolgt werden. Aus dem Verlauf des Fehlstellenaufbaus über ca. 1% der Bruchzyklenzahl kann eine Bruchvorhersage gemacht werden.

Die Möglichkeiten der Schadensvorhersage mit Hilfe der ortsaufgelösten Positronenspektroskopie soll anhand eines ferritischen und eines austenitischen Stahls an kreisförmig taillierten Zugproben vorgestellt werden.

MM 38.2 Di 10:45 TU H111

Measurement of crack growth rate of magnesium alloy AZ31 — •Zuzana Zuberova[1], Ludvik Kunz[2], Ralph Jörg Hellmig[1], and Juri Estrin[1] — [1]Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678 Clausthal-Zellerfeld — [2]Academy of Sciences of the Czech Republic, Institute of Physics of Materials, Brno, Czech Republic

In this work the crack growth rate for magnesium alloy AZ31 was investigated. This alloy was produced as squeeze cast material with low porosity and with a grain size of about 450 μm. For determining the crack growth rate a resonant machine (Amsler 5100) was used. The experiment was run in load amplitude control by symmetrical sinusoidal load cycles with a frequency of 145 ± 5 Hz. The crack propagation was investigated by optical microscopy, showing multiple branching of the magistral crack. Paris equation was shown to hold despite a large scatter in experimental data. A threshold intensity factor of $K_{ath} = 0.8$ MPa·$m^{1/2}$ was determined.

MM 38.3 Di 11:00 TU H111

An ab initio study of the connection between elasticity and crack formation — •Petr Lazar[1], Raimund Podloucky[1], and Walter Wolf[2] — [1]Institute for Physical Chemistry of Univ. Vienna, Liechtensteinstrasse 22A, A 1090 Vienna, Austria — [2]Materials Design s.a.r.l., 44, av. F.-A. Bartholdi, 72000 Le Mans, France

The connection between elasticity and crack formation is of long-time interest. The conceptual problem is that the elastic response to an external load is nonlocal because the energy dissipates over the whole material, whereas the crack formation energy is localized around the crack. Our crucial ansatz is, that at a critical load or crack size, elastic response and crack formation are in equilibrium and now the elastic energy is also localized. For single crystals we studied the formation of cracks of type 1 for which the crack is initialized by cleaving the material. The two extreme cases were considered: 1) no atomic relaxation after crack formation (ideal brittle cleavage) [1]; 2) full relaxation in terms of a perfect elastic response. From ab initio calculations [2] for a variety of materials and crack directions we obtain the energy as a function of crack size which serves for the derivation of model parameters. Based on this combination of ab initio data and analytic modelling we arrive at the equation C = a G, in which C is an elastic modulus, G is the cleavage energy, and a is a parameter of local character.

[1] Rose et al., PRB 28,1835 (1983)
[2] G. Kresse and J. Joubert, PRB 59,1758 (1999)

Supported by the Austrian Science Fund (Science College W4).

MM 38.4 Di 11:15 TU H111

Spannungsabhängigkeit von Aktivierungsvolumen und Aktivierungsenergie von plastisch verformtem Strontiumtitanat unterhalb Raumtemperatur — •Dieter Brunner — Max-Planck-Institute für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart

Die Temperaturabhängigkeit der Kritische Schubspannung von Strontiumtitanat ist unterhalb Raumtemperatur (RT) durch drei unterschiedliche Bereiche gekennzeichnet. In Druckversuchen (Druckrichtung < 001 >) wurden in den drei Bereichen die Parameter thermisch aktivierter Versetzungsbewegung, Aktivierungsvolumen und Aktivierungsenergie, bestimmt. Die dazu benötigte Dehnratenempfindlichkeit (SRS) wurde sowohl direkt aus Spannungsrelaxationsversuchen (SRV) als auch mit Hilfe eines speziellen Verfahrens [1] aus SRV bestimmt, welches Aussagen zum thermischen Aktivierungsprozess und präexponentiellen Faktor der Arrheniusgleichung ermöglicht. Auch für SRS und damit auch für Aktivierungsvolumina und Aktivierungsenergien wurde drei Bereiche gefunden, was auf unterschiedliche Versetzungskerne oder verschiedene Moden der Versetzungsbewegungen hinweist. Die Grösse der gefundenen Aktivierungsparameter legt nahe, dass im Bereich unmittelbar unterhalb RT bis etwa 230 K Stufenversetzungen wie etwa in kfz Metallen dominieren, während dies im Tieftemperaturbereich (<200 K) eine den krz Materialien zugrundeliegende Schraubenversetzungsbewegung ist, bestimmt durch thermisch aktivierte Kinkpaarbildung. Der Zwischenbereich (200 K <T<230 K) ist dann durch einen Übergang zwichen beiden Versetzungstypen gekennzeichnet. [1] D. Brunner, J. Diehl: phys.stat.sol. (a) 104 (1987) 145-155.

MM 39 Mechanische Eigenschaften II

Zeit: Dienstag 11:30–12:15 Raum: TU H111

MM 39.1 Di 11:30 TU H111

EFFECT OF MECHANICAL STRESS FIELDS ON RECRYSTALLIZATION OF AN Al-Mg ALLOY — •Carmen Schäfer and Myrjam Winning — Institut für Metallkunde und Metallphysik, RWTH Aachen. Kopernikusstr. 14, 52056 Aachen

The motion of grain boundaries is the key phenomenon of recrystallization and grain growth and dominates the evolution of texture and microstructure, i.e. the macroscopic physical and mechanical properties of a material, in particular of a part in service. Recently it could be experimentally shown that mechanical stresses can influence the dynamical behavior of individual, planar grain boundaries. From these results, we can conclude that there must be also effects of mechanical stress fields on the behavior of grain boundaries in polycrystalline materials. Consequently, the aim of this study was to demonstrate the effect of mechanical stresses on the recrystallization behavior of an Al-2

MM 39.2 Di 11:45 TU H111

Dynamic recrystallization of torsion deformed NiAl — •Burghardt Klöden[1], Werner Skrotzki[1], Carl-Georg Oertel[1], and Erik Rybacki[2] — [1]Institute of Structural Physics, Division of Metal Physics, Dresden University of Technology, D-01062 Dresden, Germany — [2]Geo Research Centre Potsdam, D-14473 Potsdam, Germany

Samples of the binary intermetallic compound NiAl with different initial textures were deformed in torsion in a Paterson type rock deformation machine under hydrostatic pressure of 400 MPa and at a constant maximum strain rate of $10^{-4}s^{-1}$ at temperatures between 800K and 1300K. The maximum shear strain after up to 3 revolutions was 9 to 18. High temperature torsion as one of the modes of severe plastic deformation has been used, because due to a gradient in shear strain across the sample, the continuous development of microstructure and texture with strain can be investigated. Experimental methods included the use of the EBSD technique and high energy synchrotron radiation. The mechanisms of microstructure and texture development will be discussed with emphasis being put on dynamic recrystallization phenomena.

MM 39.3 Di 12:00 TU H111

Dynamic Recrystallization under Transient Deformation Conditions — •Matthias Frommert and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, D-52056 Aachen, Germany

Dynamic recrystallization (DRX) is a softening process that occurs during high temperature deformation and, therefore, affects the strength of a material. Dependent on the deformation parameters and initial grain size the typical DRX flow curve is known to display either a single-peak or multiple-peak behaviour before attaining steady-state stress. Transient deformation conditions such as changes of strain rate or temperature not only influence the shape of the flow curve but also the dynamically recrystallized grain size which is dependent on the steady-state flow stress.

Compression tests were performed with an austenitic steel Alloy 800H to investigate the mechanisms of DRX. Microstructure and texture were analysed using optical microscopy, SEM and X-ray diffraction, respectively. When the true strain rate is changed at a defined strain during the experiment the dynamically recrystallized grain size readjusts within a short strain interval as evident from the resulting change of steady-state flow stress. The inverse pole-figures demonstrate that during the early stages of high temperature deformation a typical deformation texture evolves which is randomized by the onset of DRX.

MM 40 Diffusion I

Zeit: Dienstag 10:30–11:30 Raum: TU H2038

MM 40.1 Di 10:30 TU H2038

Simulation of Internal Oxidation of Engineering Alloys under Industrial Process Conditions — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt

Internal oxidation is of great technical importance as effective dispersion-hardening method or undesirable side effect to steel heat treatments. Reaction kinetics is usually described by Wagner's theory that is designed for laboratory conditions but does not sufficiently cover industrial operations due to the restriction to homogeneous concentration distributions of the less noble component M within the matrix metal, isobaric and isothermal processes. In order to overcome these limitations, a computer model based on iterative solution of Fick's law for the in-diffusion of oxygen with arbitrary initial distribution of M atoms is proposed. The solubility product and the stoichiometry factor of the precipitating oxide define the mass balance relationship. For homogeneously dissolved M atoms and isothermal-isobaric reaction conditions, it is shown that the results agree excellently with Wagner's theory and experimental data. Heterogeneous M distributions as well as nonisobaric and/or nonisothermal internal oxidation are accessorily covered by the new model. Illustrative processes are calculated and the results are discussed in detail.

MM 40.2 Di 10:45 TU H2038

Hyperfein Wechselwirkung von implantierten ^{111}Cd-Sonden im Hf_2Au Gitter — •P. Wodniecki[1,2], M. Uhrmacher[2], A. Kulinska[1,2], B. Wodniecka[1] und K.P. Lieb[2] — [1]IFJPAN, Krakow, Polen — [2]II. Physikalisches Institut, Universität Göttingen

Wir berichten über PAC Messungen der elektrischen Feldgradienten, die man mit der Sonde ^{111}In/^{111}Cd im Hf_2Au Gitter findet. Dieses Gitter bildet sich in einer einfachen tetragonalen $C11_b$ Struktur, deren Prototyp $MoSi_2$ ist. Es handelt sich dabei um die D^{17}_{4h}-Raumgruppe. Zwei Au-Atome und vier Hf-Atome bilden die Einheitszelle. Alle Plätze [Hf: 4(e)4mm, Au: 2(a) 4/mmm] sind achsialsymetrisch bezgl. der c-Achse und der EFG Tensor ist diagonal an jedem Gitterplatz der Struktur.

Der Gitterplatz der implantierten In-Sonden ist in diesem Gitter unvorhersehbar, da man In als Verunreinigung in der Hf_2Au Matrix ansehen muss. Als weitere Unwägbarkeit könnte sich der eingenommene Gitterplatz der PAC-Sonden mit der Temperatur ändern. Diesen Fall haben wir bei der Untersuchung von $TiPd_2$ beobachtet, das in der gleichen Struktur vorliegt [1]. Daher war das Hauptanliegen der Untersuchung, die Hyperfein-Wechselwirkungsparameter in einem weiten Temperaturbereich zu messen, um die besetzten Gitterplätze und mögliche Platzwechsel zu beobachten.

[1] P. Wodniecki, B. Wodniecka, A. Kulinska, M. Uhrmacher, K.P. Lieb, J.Alloys and Compounds 385 (2004) 53.

MM 40.3 Di 11:00 TU H2038

Grain Boundary Radiotracer Diffusion and Segregation of Fe and Ni in Polycrystalline Cu — •Jens Ribbe, Sergiy Divinski, Guido Schmitz, and Christian Herzig — Institut für Materialphysik, Universität Münster,Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

^{59}Fe and ^{63}Ni grain boundary (GB) diffusion in high-purity Cu was measured by the radiotracer method combined with mechanical sectioning technique in an extended temperature interval. At higher temperatures the conditions of Harrison's B kinetics were satisfied and the triple product $P = s \cdot \delta \cdot D_{\mathrm{gb}}$ of the segregation factor s, GB width δ, and the GB diffusivity D_{gb} was determined at selected temperatures. Performing GB diffusion measurements at lower temperatures under the C regime conditions, the GB diffusion coefficient D_{gb} was directly measured. Using the estimate of the GB width deduced from GB self-diffusion measurements on FCC metals, $\delta \approx 5 \cdot 10^{-10}$ m, the segregation factor s of Fe was determined as $s = P/\delta D_{\mathrm{gb}}$. Fe reveals high segregation and very slow diffusivity D_{gb} in Cu high-angle GBs. However, the measured triple product P^{Fe} for Fe GB diffusion is by orders of magnitude larger than the GB diffusivity P^{Ni} of Ni. The main reason is the strong GB segregation of Fe in Cu.

MM 40.4 Di 11:15 TU H2038

Nickel Radiotracer Diffusion in B2 Ordered $Ni_{50-x}Fe_xAl_{50}$ Alloys — •Sergiy Divinski[1], Frank Hisker[1], Wolfgang Löser[2], Ulf Södervall[3], and Christian Herzig[1] — [1]Institut für Materialphysik, Universität Münster, Germany — [2]IFW Dresden, Dresden, Germany — [3]Department of Physics, Chalmers University of Technology,Göteborg, Sweden

Ni bulk diffusion was measured in a series of B2 ordered $Ni_{50-x}Fe_xAl_{50}$ alloys. The ^{63}Ni radioisotope in combination with the serial sectioning technique was applied at higher temperatures and the secondary ion mass spectrometry (the ^{64}Ni isotope) was used in a low temperature range. In the temperature interval from 1050 to 1500 K, well-type Arrhenius temperature dependencies were established for all studied compositions. As the Fe content x in the $Ni_{50-x}Fe_xAl_{50}$ ternary alloys increases, the Ni diffusivity generally increases. The activation enthalpy Q of Ni diffusion changes strongly non-monotonously in the ternary alloys between the binary end-members NiAl and FeAl revealing a pronounced minimum at the $Ni_{40}Fe_{10}Al_{50}$ composition and a conspicuous maximum around the $Ni_{25}Fe_{25}Al_{50}$ composition. The latter indicates additional ordering (e.g. of the $L2_1$ type) in the corresponding alloys.

MM 41 Diffusion II

Zeit: Dienstag 11:30–12:30 Raum: TU H2038

MM 41.1 Di 11:30 TU H2038

Wasserstoff gebunden an Leerstellen in Al-Werkstoffen: Nachweis mit Positronenvernichtung? — •Torsten E.M. Staab, Michael Röbel, Christiane Zamponi und Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn, Germany

Aluminiumwerkstoffe erhalten ihre Festigkeit durch Ausscheidungen ihrer Legierungselemente, die die Versetzungsbewegung effektiv behindern. Kommt es bei Ermüdungsexperimenten unter korrosivem Medium (simuliertes Meerwasser) zu einer Rissbildung, kann Wasserstoff aus der Lösung in die Probe diffundieren und dort an Leerstellen, die durch Jog-Dragging entstanden sind, eingefangen werden. Ab-initio Rechnung zeigen, dass Wasserstoff in Leerstellen eine Bindungslänge zu den Nachbaratomen eingeht, die in etwa dem Abstand des adsorbierten Wasserstoffatoms an Al-Oberflächen entspricht. So maskiert Wasserstoff am Rand die Leerstellen für die Positronenvernichtung nicht, andererseits könnte er durch seine negative Ladung den Einfangkoeffizienten sogar deutlich erhöhen. Rechnungen zeigen, dass der Wasserstoff über eine Änderung der Impulsverteilung mit Positronenvernichtung nachgewiesen werden könnte.

MM 41.2 Di 11:45 TU H2038

Schallgestützte Strahlenschädigung — •Christine Negrini, Poornima Anbalagan, André Engelbertz, David Tyler Hartman und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms-Universität zu Bonn

Strahlenschäden und die Folgereaktionen sind nicht nur in der Physik, sondern auch in der Biologie, Chemie und Medizin von besonderem Interesse. Für die hier vorgestellten Messungen diente Quarzglas als Modellsystem. Die Strahlenschädigung wurde zum einen durch reine Protonenbestrahlung und zum anderen durch Protonenbestrahlung bei gleichzeitigem Einstrahlen von unterschwelligem Ultraschall erzeugt. Zur Untersuchung der unterschiedlichen Effekte wurden die beiden Proben mit Hilfe der Spannungsoptik, der ortsaufgelösten Positronenannihilation und optischer Absorptionsspektroskopie bis zu Wellenlängen von 180 nm untersucht. Im Vergleich der Ergebnisse zeigte sich ein signifikanter Unterschied zwischen den Proben, die nur mit Protonen bestrahlt wurden, und den Proben, die mit Protonen und Ultraschalleinstrahlung behandelt wurden.

MM 41.3 Di 12:00 TU H2038

Magnetfeld induzierte Diffusion von Positronen in Metallen — •Thorsten Müller, Matz Haaks und Karl Maier — Helmholtz - Institut für Strahlen- und Kernphysik der rheinischen Friederich- Wilhelms Universität zu Bonn

Die Empfindlichkeit der Positronen-Annihilation-Spektroskopie auf Fehlstellen ist Raten- oder Diffusionslimitiert. Bei niedrigen Fehlstellenkonzentrationen wird der Positroneneinfang durch die Diffusion des Positrons limitiert. Die Wahrscheinlichkeit, eine Fehlstelle zu finden, hängt dabei wesentlich vom Diffusionsvolumen ab. Beeinflusst von der Lorentz-Kraft, bewegt sich das Positron während der Diffusion auf Spiralbahnen, wodurch sich das Diffusionsvolumen beeinflussen lässt.

Der Einfluss homogene Magnetfelder bis zu 5 Tesla wurden untersucht. Als Probe diente ein leicht verformter Kupferzylinder mit ^{68}Ge Quelle als Positronenquelle. Die feldstärkeabhängigen Messungen wurden bei verschiedenen Temperaturen zwischen 77 K und 340 K durchgeführt. Bei konstanter Temperatur und steigendem Magnetfeld zeigt sich eine Abnahme des S-Parameters. Daraus kann in leicht verformten Cu auf eine Abnahme des Diffusionsvolumens geschlossen werden.

MM 41.4 Di 12:15 TU H2038

Messungen an thermisch belastetem Messing mit einem ortsauflösenden Doppler-Koinzidenzspektrometer am intensiven Positronenstrahl NEPOMUC — •Martin Stadlbauer[1], Christoph Hugenschmidt[1,2], Klaus Schreckenbach[1,2] und Benno Strasser[2] — [1]Technische Universität München, Physikdepartment E21, James-Franck-Str., 85748 Garching — [2]Technische Universität München, ZWE FRM-II, Lichtenbergstr. 1, 85748 Garching

Im Rahmen einer Diplomarbeit wurde am intensiven Positronenstrahl NEPOMUC des FRM-II ein ortsauflösendes Doppler-Koinzidenzspektrometer aufgebaut. Dieser Beitrag stellt das Spektrometer kurz vor und zeigt an Hand einiger ortsaufgelöster Messungen an thermisch behandeltem Messing die experimentellen Möglichkeiten. Im Spektrometer wird der intensive Positronenstrahl auf etwa 2 mm fokussiert. Die $20 \times 20\,mm^2$ abmessende Probe wird dabei auf 0 bis -20 kV gelegt und kann im Vakuum senkrecht zur Strahlrichtung verfahren werden, um ortsaufgelöste Messungen zu ermöglichen. Die entstehende Annihilationsstrahlung wird durch zwei koinzident ausgelesene Germaniumdetektoren nachgewiesen, so dass große Doppler-Verschiebungen, die hohen Elektronenimpulsen entsprechen, gemessen werden können. Dadurch wird eine starke Untergrundunterdrückung erreicht, die eine elementspezifische Messung möglich macht.

MM 42 Hauptvortrag Mike Finnis (Max-Born Preisträger)

Zeit: Dienstag 14:00–14:30 Raum: TU H1058

Hauptvortrag MM 42.1 Di 14:00 TU H1058

Atomic size matters — •Mike Finnis — Atomistic Simulation Center, Department of Physics and Astronomy, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK — Träger des Max-Born-Preises

"Atomic size" is a concept often referred to by metallurgists when talking about the rules governing the location or behaviour of impurities, but it has been treated with some suspicion by solid-state theorists who do first-principles calculations. I will describe some recent calculations that address a very old problem: why is Cu embrittled by a few tens of parts per million of Bi? There has been some controversy about this kind of effect, with a general belief that it is electronic in origin, whereby the impurity draws electrons from Cu-Cu bonds and weakens them. By means of first-principles calculations we have found [1] that on the contrary, in the case of Bi in Cu the effect can be explained by the larger atomic size of Bi and its insolubility in Cu, and electron transfer appears to be insignificant.

[1] Schweinfest, R., A.T. Paxton and M.W. Finnis, Bismuth embrittlement of copper is an atomic size effect. Nature, 2004. In press.

MM 43 Symposium Tomographic Methods in Materials Research Hauptvortrag Wolfgang Treimer

Zeit: Dienstag 14:45–15:15 Raum: TU H1058

Hauptvortrag MM 43.1 Di 14:45 TU H1058

Absorption- and phase-based imaging signals for neutron tomography — •Wolfgang Treimer — Unversity of Applied Sciences (TFH) Berlin, FB II, D - 13353 Berlin

Thermal and cold Neutrons are a perfect tool to investigate massive and large (several cm3) samples by means of computerized tomography (CT). The main interaction to visualize structures in samples is absorption, similar to x-rays in medicine or material research. Based on absorption new techniques such as energy dependent CT or real time CT have gained importance within the last years and were used to show e.g. the movement of pistons in engines. Absorption, however, is not the only interaction that can be used for computerized tomography. Other interactions such as interference effects, so-called phase based interactions, were exploited for CT to visualize details in samples that could not be detected by absorption. Phase contrast imaging was first applied to x-ray CT, but soon it was also applied to neutron CT. Based on the same interaction, refraction and ultra small angle scattering of neutrons were studied and successfully applied to neutron tomographic investigations of samples. These new imaging signals (refraction and ultra small angle scattering) require entirely different techniques, different experimental set ups (high resolution double crystal diffractometer)and data evaluation, to detect these signals and separate them from absorption and noise. Using absorption and phase-based signals the length scale of tomography with neutrons is more than five orders of magnitude, which covers a large field of non-destructive testing in material research and fundamental physics.

MM 44 Symposium Tomographic Methods in Materials Research

Zeit: Dienstag 15:15–16:15 Raum: TU H1058

MM 44.1 Di 15:15 TU H1058

In-situ Synchrotron X-ray Tomography Investigation of Creep Damage — •Anke Rita Pyzalla[1], Bettina Camin[2], Heinz Kaminski[1], Andreas Kottar[1], Andrea Pernack[2], Karolina Zimnik[1], Thomas Buslaps[3], Marco di Michiel[3], Elodie Boller[3], and Walter Reimers[2] — [1]TU Wien, Institute of Material Science and Technology, 1040 Wien, Austria — [2]Institute of Material Sciences and Technologies, 10587 Berlin, Germany — [3]ESRF, 38043 Grenoble, France

Using a novel miniature creep device the development of creep pores, pore agglomeration and crack growth could be investigated in-situ at high temperature for the first time using synchrotron X-ray tomography. The evolution of the pore volume, pore size and their dependency on temperature and creep stress is presented. The results of the experiments further reveal characteristic differences of the damage evolution for materials containing soft and hard second phase particles.

MM 44.2 Di 15:35 TU H1058

Materials analysis by joined microfocus computer tomography (μCT) and 3D Photogrammetry — •Matthias Schulze, Michael Nöthe, Bernd Kieback, and Hans-Gerd Maas — Technische Universität Dresden

The most important drawback in the theoretical description of sintering processes is the lack of a sufficient incorporation of cooperative material transport processes. This results in an inconsistence of the predicted and observed shrinkage behaviour of real sintered specimens. The first method to gain data necessary to develop a theory of cooperative material transport processes is microfocus computer tomography (μCT) joined with 3D photogrammetric image analysing to determine the particles and their motions. With methods based on subvoxel image analysing particles are detected automatically and their surface is modelled with subvoxel precision. To determine the spatial dynamic during the sintering process tracking and matching algorithms are implemented to trace single objects. These data proved the rotation of particles and allowed to determine geometrical and topological features like shape parameter, contact partners and interparticle contact area. These results give hints on the nature of the particle rearrangement and the characteristics of the sintering process. In addition the versatility of 3D photogrammetric image analysis will be shown by means of the development of cracks in concrete.

MM 44.3 Di 15:55 TU H1058

Special features of tomography with cold neutrons — •Nikolay Kardjilov[1], André Hilger[1,2], Ingo Manke[1,3], Markus Strobl[1,2], Wolfgang Treimer[1,2], and John Banhart[1] — [1]Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin — [2]Technische Fachhochschule Berlin, Luxemburger Straße 10, 13353 Berlin — [3]TU-Berlin, Straße der 17 Juni 135, 10623 Berlin

Cold neutrons interact stronger with most materials than thermal neutrons. Therefore the image contrast and the element detection sensitivity in tomography investigations can be improved by using cold neutrons. In contrast to neutron tomography with thermal neutrons, cold neutron tomography has its own specifics which should be taken into account in when processing experimental data. The influence of the Bragg-cut-off , beam hardening and spectral effects lead to a complicated image formation. Typical examples of cold neutron tomography experiments will be discussed and analyzed.

MM 45 Symposium Tomographic Methods in Materials Research Hauptvortrag Eberhard Lehmann

Zeit: Dienstag 16:30–17:00 Raum: TU H1058

Hauptvortrag MM 45.1 Di 16:30 TU H1058

Neutron tomography as tool for applied research and technical inspection — •Eberhard H. Lehmann and Peter Vontobel — Paul Scherrer Institut, CH-5232 Villigen PSI

Similar to the imaging with X-ray, neutron imaging systems have been shifted more and more from film exposure towards direct digital detection in the last decade. This approach enables the option for tomography because the image content is measured and understood as dataset now. With the help of mathematical algorithms it becomes possible to derive the necessary information about the full three-dimensional volume from a set of projections from different viewing angles. Neutron tomography with best performance requires a strong and well collimated neutron beam. Such beam lines for either thermal or cold neutrons are available at reactor based sources (FRM-2, HMI, ILL) or at spalltion sources (PSI). The beam geometry for neutrons is in the best case parallel ones, delivering a sharp 1:1 image of the object under investigation. Therefore, the detector resolution is responsible for the tomography resolution generally. In practical reality, objects with outer dimensions up to 40 cm can be inspected with a resolution of 0.1 mm. This compares well with some X-ray tomography systems. However, the application fields are completely different. Neutrons have the advantage to penetrate most metals (especially heavy ones) very efficiently and to detect hydrogenous compounds very sensitively. Therefore, neutron tomography has application fields in moisture detection, test of adhesive connections, structure analysis for soil and geology and the non-invasive investigation of samples from our cultural heritage.

MM 46 Symposium Tomographic Methods in Materials Research

Zeit: Dienstag 17:00–18:00 Raum: TU H1058

MM 46.1 Di 17:00 TU H1058

Detection of texture alteration in Al parts using Neutron Computed Tomography — •Burkhard Schillinger[1], Johannes Brunner[1], Roland Gähler[2], Martin Mühlbauer[1] und Michael Schulz[1] — [1]TU München - FRM-II, 85747 Garching — [2]Institut Laue-Langevin, F-38042 Grenoble

Neutron Computed Tomography has been developed to higher and higher sensitivity during the past years. At the research reactor FRM II of Technische Universitaet Muenchen, texture alterations caused by stress in Aluminium parts have been detected for the first time in a large measuring volume using Neutron Computed Tomography. By mechanical deformation, local stress and texture alterations were introduced into Aluminium plates. The altered texture lead to increased small angle scattering, which causes more beam attenuation in large distance between sample and detector. The new method can be used as large-volume pre-examination for quantitative measurements with the Neutron Stress Spectrometer in order to predetermine the areas which should be examined more closely. A Neutron Tomography of a sample of 20 cm size can be measured in about two hours, while a blind scan of the volume on the stress spectrometer may take several days. By preselection of the volumes to be measured, the efficiency of the stress spectrometer can be increased by orders of magnitude.

MM 46.2 Di 17:20 TU H1058

Neutron tomography on fuel cells — •Ingo Manke[1,2], Markus Strobl[1,3], Nikolay Kardjilov [1], André Hilger[1], Joachim Scholta[4], Werner Lehnert[4], Wolfgang Treimer[1,3], and John Banhart[1,2] — [1]Hahn-Meitner-Institut Berlin, Glienicker Str 100, D-14109 Berlin — [2]Technische Universität Berlin, Straße der 17.Juni 135, D-10623 Berlin — [3]Technische Fachhochschule Berlin, Luxemburger Straße 10, 13353 Berlin — [4]Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Industriestr. 6, 70565 Stuttgart

Neutrons can penetrate thick metal components while they are very sensitive to hydrogen and other light elements. Therefore neutron imaging can be used as a tool for non-destructive analysis of operating fuel cells. They allow for an analysis of internal cell processes, specifically, the formation and transportation of water throughout the cell. In a low temperature fuel cell (PEMFC) water is produced as a byproduct of the conversion of hydrogen fuel to electrical energy and exists mostly in liquid form as a result of the low operating temperature. However, the development of too much water can disturb the hydrogen/water flow yielding a breakdown in the output power. Thus an efficient water management is very important in the effort to optimize fuel cell energy production. In-situ neutron radiography has been used to investigate the water development in fuel cells applying realistic profiles of power consumption which are, e.g., rapid changes of the power profile (accelerating and breaking in case of an automotive application) and repeated start/shut down cycles as they appear e.g. in portable systems. A special problem is the accumulation of water at the bottom of the fuel cell due to gravity.

MM 46.3 Di 17:40 TU H1058

Neutron radioscopy of a running combustion engine — •Johannes Brunner — FRM-II, 85747 Garching, Lichtenbergstr. 1

Dynamic neutron radiography is a non-destructive testing method, which made big steps in the last years. Depending on the neutron flux, the object and the detector a time resolution down to a few milliseconds is possible. In the case of repetitive processes the object can be synchronized with the detector and better statistics in the image can be reached by adding radiographies of the same phase. By delaying the trigger signal a radiography movie can be composed with a time resolution down to 100 mys. A combustion engine is an ideal sample for the explained technique, because the motor block of metal is relatively easy to penetrate, while oil and fuel attenuate the thermal neutron beam much stronger. After various experiments at ILL and PSI the first measurements at the new neutron source FRM-II started.

MM 47 Mechanische Eigenschaften III

Zeit: Dienstag 14:45–16:00 Raum: TU H111

MM 47.1 Di 14:45 TU H111

Texture induced plastic anisotropy of rolled molybdenum sheets — •Ingwar Hünsche[1], Carl-Georg Oertel[1], Werner Skrotzki[1], Wolfram Knabl[2], Alexander Lorich[2], and Joachim Resch[2] — [1]Institut für Strukturphysik, Technische Universität Dresden, — [2]PLANSEE Aktiengesellschaft, A-6600 Reutte/Tyrol, Austria

The microstructure, texture and mechanical properties of molybdenum sheets produced by PLANSEE AG in different rolling processes were investigated by orientation imaging in the scanning electron microscope, X-ray diffraction and tensile tests. Tensile tests were done in different directions of the rolled sheets. Results on the mechanical properties will be correlated with texture and microstructure of three different type of sheets. The texture of the sheets is characterized by components lying on the α - and γ -fibre typical for bcc metals (α-fibre: $\langle 110 \rangle \parallel$ rolling direction, γ-fibre: $\langle 111 \rangle \parallel$ rolling plane). The different production processes used lead to changes in intensity of the components and thus to varying mechanical properties. The aim is to correlate microstructure and texture with mechanical properties in order to optimize the deep-drawability of the molybdenum sheets by modifying the production process.

MM 47.2 Di 15:00 TU H111

Control of the Porous Structure of Aluminium Foams — •B. Matijasevic-Lux[1], Th. Lonkai[2,3], S. Fiechter[2], N. Wanderka[2], P. Schuber-Bischoff[2], and J. Banhart[2,3] — [1]Institute of Materials Sciences and Technology, Technical University Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany — [3]Institute for Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

A high rigidity combined with a low weight makes aluminium foams a very promising material for modern engineering. The quality of metal foams depends on the homogeneity of the porous structure. We succeeded in controlling the homogeneity of the porous structure of aluminium foams by heat treatment of the blowing agent TiH_2 under air. The TiH_2 powder was characterised by thermal analysis, mass spectrometry, X-ray and neutron diffractometry (XD,ND) and transmission electron microscopy (TEM). Mass spectrometry showed that hydrogen release from as-received TiH2 powder in argon shows two decomposition peaks while after pre-treatment in air the first decomposition stage is eliminated and the second shifted to higher temperatures depending on the nature of heat treatment. The elimination of the first decomposition improved the homogeneity of the porous structure of the metal foam significantly. The effect was attributed to oxide layers around the cores of TiH2 particles, observed by a combination of XD, ND and TEM experiments, which build up during pre-treatment and act as diffusion barriers to hydrogen. The oxide layers consists of two different titanium oxides, namely tetragonal TiO_2 and hexagonal Ti_3O of about 100 nm thickness.

MM 47.3 Di 15:15 TU H111

Finite-Elemente Berechnung des orientierungsabhängigen Kriechverhaltens von Nickel-Basis Superlegierungen. — •Yegor Rudnik, Johannes Preussner, Rainer Völkl und Uwe Glatzel — Metallische Werkstoffe, Universität Bayreuth, Ludwig-Thoma-Str. 36b, 95447 Bayreuth

Wichtig für das Verhalten einkristalliner Bauteile ist die Berücksichtigung der starken Anisotropie der Eigenschaften. Für die Untersuchung des Kriechverhaltens einer Nickel-Basis Superlegierung wurden drei Finite-Elemente Modelle entwickelt, die die Kriechvervormung des Materials in drei Kristallrichtungen [001], [011] und [111] simulieren. Als Kriechgesetz wurde das Gesetz von Norton angewandt. Das anisotrope Verhalten der Legierung wird anhand der Spannungsverteilung und der Geometrieänderung der Struktur im Laufe der Zeit erklärt.

MM 47.4 Di 15:30 TU H111

Mechanical properties of macro-alloyed, single-phase D03-ordered iron aluminides — •Johannes Deges — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str.1 40237 Düsseldorf

Iron aluminides exhibit an excellent corrosion and oxidation resistance in the range of the operating temperatures of steam turbines. Therefore, they possess a high potential as a low cost alternative to conventional ferritic, martensitic or austenitic steels. For the application as a structural material the improvements of the mechanical properties, such as room temperature ductility and strength at temperatures above 600°C are necessary. In the framework of a systematic alloy development different Fe3Al-based alloys with ternary additions of transition metals: Ti, V, Nb, Ta, Cr, Mo, W, Mn, Co, Ni, Cu have been produced by vacuum induction melting. The influence of the alloying elements on the mechanical properties like warm strength and plastic elongation at room temperature have been investigated in the as-cast condition and after a defined D03-ordering heat treatment. The first results show that low concentrations of the alloying elements have a strong influence on the stress-strain behaviour as well as the fracture mode.

MM 47.5 Di 15:45 TU H111

Materialmodell zur Beschreibung des Kriechverhaltens einkristalliner Metalle basierend auf Versetzungsdichten. — •Johannes Preussner[1], Yegor Rudnik[1], Holger Brehm[2], Rainer Völkl[1] und Uwe Glatzel[1] — [1]Metallische Werkstoffe, Universität Bayreuth, Ludwig-Thoma-Str. 36b, 95447 Bayreuth — [2]Fraunhofer IWM, Wöhlerstraße 9-13, 79108 Freiburg

Einkristalline Bauteile weisen in ihren Eigenschaften eine starke Anisotropie auf. Ein Materialmodell wird vorgeschlagen, welches das Kriechverhalten mit Hilfe von Entwicklungsgleichungen der Versetzungsdichten auf den einzelnen Gleitsystemen beschreibt. Eine Wechselwirkungsmatrix bestimmt dabei den Einfluss eines Gleitsystems auf das andere. Ein kubisch-flächenzentriertes Gitter wird betrachtet und es wird angenommen, dass die Gleitung auf oktaedrischen und kubischen Gleitebenen mit Burgersvektor a/2 [110] stattfindet. So müssen neun unabhängige Parameter für die Wechselwirkungsmatrix unterschieden werden. Das Materialmodell wurde in ein FEM-Programm eingebettet, um die Kriecheigenschaften zweiphasiger einkristalliner Nickelbasissuperlegierungen zu simulieren.

MM 48 Mechanische Eigenschaften IV

Zeit: Dienstag 16:30–17:45 Raum: TU H111

MM 48.1 Di 16:30 TU H111

Dislocation processes in a peak to overaged γ'-strengthened nickel base alloy studied by in situ TEM tensile tests — •Dietmar Baither[1], Volker Mohles[2] und Eckhard Nembach[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster — [2]Institut für Metallkunde und Metallphysik, Rheinisch-Westfälische Technische Hochschule, 52056 Aachen

The commercial nickel base alloy NIMONIC PE16 is strengthened by nanoscale spherical coherent precipitates of the γ'-intermetallic phase Ni_3(Al, Ti). Maximum strength is attained in the peak-aged state. In the transition range to the overaged state, the strength is reduced as the interaction process between dislocations and precipitates changes.

Thin foils of NIMONIC PE16 were stretched inside a TEM and the dislocation processes were observed under full load. It was found that dislocations overcome the γ'-precipitates by a combination of bypassing and shearing. Due to the $L1_2$-long range order of the γ'-precipitates two dislocations with identical Burgers vectors form a pair and glide together. The leading dislocation bypasses the γ'-precipitates and leaves Orowan loops behind. The trailing dislocation first forces the loops to shear the γ'-precipitates before it shears the precipitates itself. The dislocation configurations observed in situ in the TEM are compared with those obtained in computer simulations.

MM 48.2 Di 16:45 TU H111

Versetzungsbildung im zweiphasigen Karbonstahl C45E — •Matz Haaks, Torsten Staab und Karl Maier — Helmholtz Institut für Strahlen und Kernphysik, Nußalle 14-16, 53115 Bonn

Positonen-Annihilationsspektroskopie ist eine etablierte Methode zum Nachweis der Versetzungskonzentration über die an die Versetzung gebundenen assoziierten Leerstellen. Die Doppler-Verbreiterung der Annihilationslinie liefert dabei Information über die Konzentration der Gitterfehler. Die Analyse des Hochimpulsteils der Annihilationsstrahlung liefert eine zusätzliche Information über die chemische Umgebung des Zerstrahlungsorts. Bei einer mehrphasigen Legierung kann so bestimmt werden, in welcher Phase die Versetzungsbildung während einer plastischen Verformung hauptsächlich stattfindet. Der Karbonstahl C45E weist nach langsamem Abkühlen aus der Lösungsglühung ein feinkörniges Gefüge mit 40 % Ferrit (α-Phase) und 60 % Perlit auf. Ein Vergleich zwischen den Hochimpulsteilen von zugverformtem C45E und Graphit bzw. α-Eisen zeigt, daß eine Zunahme der Versetzungsdichte zum größten Teil in der kohlenstoffarmen α-Phase stattfindet.

MM 48.3 Di 17:00 TU H111

Interaction of screw dislocations with coherent twin-boundaries in fcc metals — •Zhao-Hui Jin[1], Karsten Albe[1], and Horst Hahn[2] — [1]TU Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23, D-64287 Darmstadt — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe

The concept of the generalized stacking fault (GSF) energy, which is generally considered to be crucial for understanding nucleation of lattice dislocations, is re- examined for various FCC metals. In this paper we study the scenario of a pure screw dislocation that starts moving towards an elementary coherent twin boundary. In order to carry plasticity further away the dislocation has to cross the twin boundary and change to a different glide plane, where it moves on. This is equivalent to a renucleation process of the dislocation, which has to be activated against constrictions of the pre-existing twin boundary. Be means of molecular dynamics simulations we can identify a crystallographically unexpected behaviour of this crossing process in Ni, Cu and Al. From the GSF energy and the driving force acting on the dislocation we can estimate the nucleation thresholds and explain the nature of bifurcated slips either into the twin lattice or along the twin plane.

MM 48.4 Di 17:15 TU H111

On the strengthening effect of precipitates with a negative stacking fault energy — •Volker Mohles — Institut für Metallkunde und Metallphysik, RWTH Aachen, 52056 Aachen

Recent atomistic computer simulations (Embedded Atom Method) by Wirth and Shim have revealed that the interaction between a dislocation and a coherent cobalt precipitate in a copper matrix differs strongly from all expectations. In literature, the interaction is described by the size mismatch (coherence stress). But the quoted simulations showed that another effect is at work in addition: while a first partial dislocation moves, it creates a stacking fault in the copper matrix. But inside the particles it actually moves the cobalt atoms near the glide plane to the more favourable hexagonal positions. The second partial cutting through the particle will restore the unfavourable cubic face centred arrangement. This effect can be described by a negative stacking fault energy inside the particles. In the present talk, the impact of this effect on the particle's strengthening effect is worked out by dislocation dynamics simulations.

MM 48.5 Di 17:30 TU H111

Investigations on the Portevin-LeChâtelier effect in Al-Mg metal-matrix composites — •Hanno Dierke[1], Stephanie Graff[2], and Hartmut Neuhäuser[1] — [1]TU Braunschweig, Inst. f. Metallphysik und Nukleare Festkörperphysik, D-38106 Braunschweig — [2]Centre des Materiaux, Ecole Nationale Superieur des Mines de Paris, F-91000 Evry

Due to their low weight and high mechanical strength AlMg alloys provide a large variety of applications as material for lightweight construction. However, the practical benefit is limited due to instabilities and inhomogeneities caused by correlated movement of dislocations during plastic deformation (PLC effect). By addition of unshearable obstacles the formation of dislocation avalanches may be prevented or at least reduced.

The metal-matrix composite (MMC) AA5754 with 2 or 5 vol% Al_2O_3 showed hardly any influence of the particles added. This could be explained by an inhomogeneous distribution of the particles during manufacturing of this MMC.
Further investigations have been performed using AA6061 as matrix material, as well as numerical modelling of the MMCs in cooperation with the Ecole des Mines, Paris.

MM 49 Grenzflächen I

Zeit: Dienstag 14:45–16:00 Raum: TU H2038

MM 49.1 Di 14:45 TU H2038

TRANSITION FROM LOW ANGLE TO HIGH ANGLE GRAIN BOUNDARIES — •Myrjam Winning — Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, 52056 Aachen

Recent experiments showed a sharp transition from low angle grain boundary to high angle grain boundary behaviour. The transition is marked by a clear change in the activation enthalpy for the grain boundary motion without any extended range. It was found that the transition angle is at the same misorientation angle for the motion of curved as well as planar grain boundaries. We would like to present an overview about the existing experimental results and theoretical considerations of the structure of grain boundaries at the transition. Especially the observation that the transition depends on the rotation axis of the grain boundary is very important, because this will influence the Brandon criterion which is often used in experiments and simulations of grain growth and recrystallization processes.

MM 49.2 Di 15:00 TU H2038

Magnetically driven selective grain growth — •Peter J. Konijnenberg, Dmitri D. Molodov, and Günter Gottstein — Institut für Metallkunde und Metalphysik, RWTH-Aachen, 52074 Aachen

Thanks to an increasing field strength of resistive wide bore high field magnets, non-ferromagnetic anisotropic materials become increasingly interesting for magnetic annealing. In these materials a driving force for grain boundary migration can be induced by an appropriately directed and suitably high external magnetic field. Thermodynamically this stems from a difference in free energy density between adjacent grains.

It is experimentally shown that annealing of locally deformed single crystals (Zn, 99.99+%) in a high magnetic field, directed along the extraordinary axis, results in growth of individual selectively grown macroscopic grains into the single crystalline host matrix. Results are discussed in terms of grain orientation and grain boundaries between these grains and the host matrix in Rodrigues-Frank parameterization. It is shown that the boundary population is clearly non-randomly distributed, independently of the crystallographic deformation direction. Furthermore, in comparison with an identical but only locally at zero field recrystallized sample series, the boundary population after magnetic annealing is clearly biased towards large disorientation angles.

On rolled, recrystallized and magnetically annealed α-Ti (CP) it is shown how a similar growth selection also affects texture evolution in a polycrystalline aggregate.

MM 49.3 Di 15:15 TU H2038

In situ measurements of grain boundary migration with a high magnetic field polarization microscopy probe — •Peter Konijnenberg, Dmitri A. Molodov, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH-Aachen, 52074 Aachen

A space resolving high magnetic field polarization microscopy probe has been developed to track grain boundaries at the surface of magnetically anisotropic metals during magnetic annealing at high field strengths. It is known from experiments that also in non-ferromagnetic anisotropic materials a sufficient driving force for grain boundary migration can be provided by external high magnetic fields.Two major advantages in this approach are a constant, adjustable and accurately known driving force and the possibility to drive plane grain boundaries with a uniform and well defined boundary structure.

In essence this probe comprises a conventional polar magneto-optic Kerr setup; a remote controlled monochromatic polarizing microscope with CCD camera in field direction and a sample chamber equipped with a resistance heated sample stage perpendicular to the field direction. With a diameter of 50mm this device fits inside bore holes of commonly accessible resistive high field magnets. The current configuration was tested for sample temperatures up to 673K and fields of 25T.

The first ever in-situ boundary migration observation during magnetic annealing is presented. Absolute boundary mobilities and energies of various asymmetric tilt and twist boundaries in high purity Zn (99.99+%) bicrystals as well as grain growth kinetics data from polycrystalline samples are discussed as a function of temperature and driving force.

MM 49.4 Di 15:30 TU H2038

Effect of Impurities on Triple Junction Motion in Aluminum. — •V.A. Ivanov[1], D.A. Molodov[1], L.S. Shvindlerman[1,2], and G. Gottstein[1] — [1]Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow Distr., 142432 Russia

The results of an investigation of the steady-state motion of grain boundary systems with triple junctions in aluminum with different magnesium content (0.1 ppm-1000 ppm) will be presented.

The migration of triple junction systems was studied *in-situ* in the temperature range between 543 and 723K using an SEM. The contact angle at the tip of the triple junctions was measured. The effect of the triple junction is discussed in term of a dimensionless criterion Λ which describes the drag influence of the triple junction on the motion of the entire boundary system.

The experiments revealed that the motion of boundary systems, studied in the entire temperature range, is controlled by grain boundary kinetics irrespective of the Mg content. The drag effect of triple junctions on grain growth in 2D systems will be discussed.

Grain boundary mobility was found to depend on material purity. The dependence of grain boundary activation parameters (activation enthalpy and pre-exponential factor) on the Mg content will be analyzed.

MM 49.5 Di 15:45 TU H2038

Untersuchung von Kornrotationen an Kupfer mittels OIM — •Markus Ziehmer[1], Carl E. Krill III[2] und Rainer Birringer[1] — [1]Universität des Saarlandes, Technische Physik, D-66041 Saarbrücken — [2]Universität Ulm, Werkstoffe der Elektrotechnik, D-89081 Ulm

Die spezifische Energie einer Korngrenze ist stark abhängig von der relativen Orientierung der angrenzenden Kristallgitter. Einkristalline Kugeln, die auf ein einkristallines Substrat gesintert sind, stellen ein geeignetes System zur Untersuchung dieser Abhängigkeit dar. Die durch die Missorientierung induzierten Drehmomente führen bei entsprechender Wärmezufuhr zur Rotation der Kugeln auf dem Substrat. Bereits in den 70er Jahren wurde mit dieser sogenannten Kugel-Platte-Methode der Nachweis erbracht, dass für spezielle Orientierungen lokale Energieminima existieren, in die die Kugeln rotieren. Im Gegensatz zur damals verwendeten Messmethode (Texturmessung) ist es heute möglich, mit der Orientational Imaging Microscopy (OIM) die Rotation einzelner Kugeln über einen sehr weiten Kugelgrößenbereich zu detektieren. Die Messung der Rotationskinetik eröffnet den Zugang, die zugrundeliegenden treibenden Kräfte und die atomaren Mechanismen der Kornrotation zu identifizieren und Rückschlüsse auf die Korngrenzenenergie zu ziehen. Wir berichten über erste Ergebnisse, die wir aus Messungen an Kupfer erhalten haben.

MM 50 Grenzflächen II

Zeit: Dienstag 16:30–17:45 Raum: TU H2038

MM 50.1 Di 16:30 TU H2038

Monte Carlo Simulation of Relaxation Processes in Grain Growth — •Dana Zöllner and Peter Streitenberger — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Materialphysik, PF 4120, D-39016 Magdeburg

A modified Monte Carlo Potts Model algorithm for single-phase normal grain growth is presented, which allows one to simulate the coarsening of the microstructure of very large grain ensembles in two and three dimensions. The temporal development of the simulated 2D and 3D grain structures exhibit, after an initial period of time, a scaling state that is characterized by a self-similar grain size distribution. A modified mean-field theory based on topological grain size correlations is presented, which yields self-similar grain size distributions that are in excellent agreement with the simulated grain structures in the scaling state. The emphasis

of the present work lies on the relaxation process to the scaling state. An algorithm is implemented which allows one to construct the spatial grain structure for a given grain size distribution. Different initial grain structures characterized by different initial grain size distributions are subjected to grain growth via the Monte Carlo Potts Model simulation. The relaxation process to the self-similar scaling state is studied by following the time development of quantities like the average grain size, the variance of the grain size distribution and topological correlations. It is tested whether the relaxation process can be described by time laws such as the stretched exponential form

MM 50.2 Di 16:45 TU H2038

Atomistic modelling of interactions between lattice dislocations and grain boundaries in body-centered cubic transition metals — •Matous Mrovec and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg

With grain sizes decreasing towards the nanometer scale, the plastic deformability of polycrystalline metals is increasingly controlled by interactions of lattice dislocations and grain boundaries. To elucidate such interactions at the atomic level, computer simulations were carried out for atomistic models of dislocations interacting with boundaries in body-centered cubic (bcc) transition metals. The interatomic interactions were described by bond-order potentials (BOP) derived from tight-binding electronic-structure theory [1]. These recently developed BOP have been applied already to simulate atomistic core structures of individual screw dislocations [2] and twin boundaries [3] in Mo, W and other bcc metals. In this contribution, BOP simulation results will be presented for atomistic structures and mechanical responses of W bicrystal models containing a twin boundary and a screw dislocation.

[1] M. Mrovec, Thesis, University of Pennsylvania (2002). [2] M. Mrovec et al., Phys. Rev. B 69 (2004) 095115. [3] T. Ochs et al., Phil. Mag. A 80, 2405 (2000).

MM 50.3 Di 17:00 TU H2038

Untersuchung der Wechselwirkung Mikrorisse-Grenzflächen zum Zweck des Grain Boundary Engineering — •Michael Marx — Universität des Saarlandes, Institut für Grundlagen der Werkstoffwissenschaft und Methodik, Geb. 43B, 66041 Saarbrücken

Die Ausbreitung kurzer Risse entscheidet über die Lebensdauer zyklisch beanspruchter metallischer Bauteile. Bis zu 90 Prozent der Lebensdauer werden in dem Stadium des Kurzrisswachstums verbraucht. Dabei können kurze Risse an Korngrenzen und Phasengrenzen in ihrem Wachstum behindert werden, bis hin zum völligen Rissstopp. Obwohl einige versetzungsbasierte Modelle zur Wechselwirkung zwischen Rissen und Korngrenzen existieren, fehlen systematische Untersuchungen der Abhängigkeiten der Wechselwirkung von der Art der Korngrenze, dem Orientierungsunterschied der angrenzenden Körner, der Eigenschaften kohärenter oder inkohärenter Phasengrenzen. Mittels Focused Ion Beam (FIB) können erstmals Mikrorisse mit genau vorherbestimmten Parametern wie Risslänge und Abstand der Rissspitze zur Korngrenze an ausgewählten Korn- und Phasengrenzen erzeugt werden und somit systematische Untersuchungen durchgeführt werden. Es werden erste In-Situ-Untersuchungen im Rasterelektronenmikroskop vorgestellt, die die Wechselwirkung FIB-initiierter Mikrorisse mit Korngrenzen zeigen. Ziel ist dabei die physikalischen Mechanismen der Wechselwirkung zu verstehen und somit die Entwicklung ermüdungsresistenter Werkstoffe durch Grain Boundary Engineering zu ermöglichen.

MM 50.4 Di 17:15 TU H2038

Influence of Tensile and Compressive Creep Deformation on Gamma/Gamma Prime Lattice Mismatch in Single Crystal Superalloys — •Weye Chen[1], Nora Darowski[2], Ivo Zizak[2], Gerhard Schumacher[2], Helmut Klingelhöffer[3], and Wolfgang Neumann[1] — [1]Humboldt University Berlin, Institute of Physics — [2]Hahn-Meitner-Institute Berlin , Structure and Dynamics — [3]Federal Institute of Materials Research and Testing, Berlin

Gamma/Gamma prime lattice mismatch has been measured in single crystal superalloy SC16 after tensile and compressive creep deformation. The measurements have bean performed at ambient temperature along [001] orientation using X-ray diffraction at BESSY. On both tensile and compressively creep-deformed specimens an orientation-dependence of lattice mismatch was observed. After tensile creep deformation an increase in lattice mismatch in the orientation parallel to the load axis and a decrease in the orientation perpendicular to the load axis were found. In the compressively creep deformed specimens, however, the lattice mismatch in both of the orientations develops in the opposite direction in comparison to that of tensile creep deformation. The relative change in lattice mismatch during compressive creep deformation is clearly smaller than that of the tensile creep-deformed specimens at comparable strains. These experimental observations are discussed on the basis of a dislocation model which involves the details of deformation nature of superalloys under tensile and compressive creep loading.

Work supported by DFG (Neu 646/5-3 and Schu 1254/3-4)

MM 50.5 Di 17:30 TU H2038

Determination of adhesion energies by using hydrogen loading. — •Eugen Nikitin, Astrid Pundt, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

Hydrogen loading of thin films leads to large mechanical stress that increases with hydrogen concentration. That results in local film detachment and buckling above a critical stress. The critical stress depends on the material as well as on the film thickness. It can be used as a measure for the adhesion energy between the film and the substrate [1]. A simple model will be presented to calculate the adhesion energy from critical stress data [2]. Adhesion energies of different metals are measured for the metal/polycarbonate interface. This work is financially supported by the DFG via grant Ki 230/30-1. [1] A. Pundt, P. Pekarski, Scr. Mat. 48 (2003) 419. [2] A. Pundt, E. Nikitin, P. Pekarsky, R. Kirchheim, Acta Mat. 52 (2004) 1579.