Metal and Material Physics Division
Fachverband Metall- und Materialphysik (MM)

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Overview of Invited Talks and Sessions

(lecture rooms H 0111, H 0107 and H 1058; Poster B)

Invited Talks

MM 1.1	Mon	9:30–10:00	H 1058	**Simple ways to complex nanowires and their application** — •Rainer Adelung, Mady Elbahri, Seid Jebril, Sebastian Wille, Michael Scharnberg
MM 2.1	Mon	10:15–10:45	H 1058	**Phase Formation in Multicomponent Monotectic Aluminum Alloys** — Djordje Mirković, Joachim Gröbner, •Rainer Schmid-Fetzer
MM 8.1	Mon	14:00–14:30	H 1058	**Microstructure tomography - an essential tool to understand 3D microstructure and local degradation effects** — •Frank Muecklich
MM 9.1	Mon	14:45–15:15	H 1058	**Atomic Diffusion in Liquid Alloys** — •Andreas Meyer, Suresh Mavila Chathoth, Winfried Petry, Tobias Unruh, Marek Koza
MM 15.1	Tue	9:30–10:00	H 1058	**Phase Transformations in Thin Films and Near-Surface Regions: Stimulation and Application** — •Dirk Carl Meyer
MM 18.1	Tue	10:15–10:45	H 0107	**Local Probing of Magnetic Properties by Electron Microscopy** — •Josef Zweck
MM 19.1	Tue	11:30–12:00	H 0107	**Atom Probe Characterization of Magnetic Thin Film Structures** — •David Larson
MM 19.2	Tue	12:00–12:30	H 0107	**Thermal stability and reaction of GMR sensor materials** — •Vitaliy Vovk, Constantin Ene, Guido Schmitz
MM 19.3	Tue	12:30–13:00	H 0107	**Solid state reactions at the interface of Heusler alloy films** — •Hans-Joachim Elmers, Andres Conca, Tobias Eichhorn, Andrei Gloskovskii, Kerstin Hild, Gerhard Jakob, Martin Jourdan, Michael Kallmayer
MM 22.1	Tue	14:00–14:30	H 1058	**Grain boundary embrittlement and cohesion enhancement in copper** — •Anthony Paxton, Alexander Lozovoi, Rainer Schweinfest, Michael Finnis
MM 24.1	Wed	14:00–14:30	H 1058	**Nanoscaled domain structures and magnetization processes in thin films** — •Volker Neu, Cristina Bran, Felix Fleischhauer, Aarti Singh, Ulrike Wolff, Ludwig Schultz
MM 24.2	Wed	14:30–15:00	H 1058	**Coherent Control of Spin Torque Dynamics** — •Hans Werner Schumacher, Santiago Serrano-Guisan, Karsten Rott, Günter Reiss, Jürgen Langer, Berthold Ocker
MM 24.3	Wed	15:00–15:30	H 1058	**KeV-He-ion bombardment induced magnetic modifications and patterning of magnetic thin film systems** — •Arno Ehresmann
MM 25.1	Wed	16:00–16:30	H 1058	**Magnetic thin film materials tailored by ion irradiation** — •Jürgen Fassbender
MM 32.1	Thu	9:30–10:00	H 1058	**Magnetic Shape Memory Alloy Films: What is different to bulk materials?** — •Sebastian Fähler
MM 33.1	Thu	10:15–10:45	H 1058	**Hydrogen Physisorption in MOFs** — •Barbara Panella, Michael Hirscher
MM 34.1	Thu	11:40–12:10	H 1058	**The Interaction of Hydrogen with Metal Surfaces: Molecular Precursors, Chemisorbed Atoms and Subsurface States** — •Klaus Christmann
MM 39.1	Thu	14:00–14:30	H 1058	**Hydrogen Chemisorption to Clusters** — •Gerd Gantefoer

MM 39.2	Thu	14:30–15:00	H 1058	**Hydrogen Storage in Light Weight Metal Hydrides: Mg-based Reactive Hydride Composites** — •M. Dornheim, U. Bösenberg, C. Pistidda, G. Barkhordarian, J. Bellosta v. Colbe, R. Bormann
MM 40.1	Thu	16:30–17:00	H 1058	**Complex Metal Hydrides** — •Michael Felderhoff

Sessions

MM 1.1–1.1	Mon	9:30–10:00	H 1058	**HV Adelung**
MM 2.1–2.3	Mon	10:15–11:15	H 1058	**SYM Phase Transformations in Metallic Melts I**
MM 3.1–3.3	Mon	11:45–12:30	H 1058	**SYM Phase Transformations in Metallic Melts II**
MM 4.1–4.5	Mon	10:15–11:30	H 0107	**Nanostructured Materials I**
MM 5.1–5.4	Mon	12:00–13:00	H 0107	**Nanostructured Materials II**
MM 6.1–6.5	Mon	10:15–11:30	H 0111	**Diffusion I**
MM 7.1–7.4	Mon	12:00–13:00	H 0111	**Diffusion II**
MM 8.1–8.1	Mon	14:00–14:30	H 1058	**HV Mücklich**
MM 9.1–9.4	Mon	14:45–16:00	H 1058	**SYM Phase Transformations in Metallic Melts III**
MM 10.1–10.6	Mon	16:30–18:00	H 1058	**SYM Phase Transformations in Metallic Melts IV**
MM 11.1–11.6	Mon	14:45–16:15	H 0107	**Nanostructured Materials III**
MM 12.1–12.6	Mon	16:45–18:15	H 0107	**Nanostructured Materials IV**
MM 13.1–13.6	Mon	14:45–16:15	H 0111	**Growth**
MM 14.1–14.7	Mon	16:45–18:30	H 0111	**Electronic Properties I**
MM 15.1–15.1	Tue	9:30–10:00	H 1058	**HV Meyer**
MM 16.1–16.4	Tue	10:15–11:15	H 1058	**SYM Phase Transformations in Metallic Melts V**
MM 17.1–17.6	Tue	11:30–13:00	H 1058	**SYM Phase Transformations in Metallic Melts VI**
MM 18.1–18.3	Tue	10:15–11:15	H 0107	**SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling I**
MM 19.1–19.3	Tue	11:30–13:00	H 0107	**SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling II**
MM 20.1–20.5	Tue	10:15–11:30	H 0111	**Electronic Properties II**
MM 21.1–21.5	Tue	11:45–13:00	H 0111	**Quasicrystals**
MM 22.1–22.1	Tue	14:00–14:30	H 1058	**HV Paxton**
MM 23.1–23.52	Tue	14:45–18:00	Poster B	**Poster session**
MM 24.1–24.3	Wed	14:00–15:30	H 1058	**SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling III**
MM 25.1–25.5	Wed	16:00–17:50	H 1058	**SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling IV**
MM 26.1–26.5	Wed	14:00–15:15	H 0107	**Liquid and Amorphous Metals I**
MM 27.1–27.5	Wed	15:45–17:00	H 0107	**Liquid and Amorphous Metals II**
MM 28.1–28.3	Wed	17:30–18:15	H 0107	**Intermetallic Phases I**
MM 29.1–29.5	Wed	14:00–15:15	H 0111	**Mechanical Properties I**
MM 30.1–30.5	Wed	15:45–17:00	H 0111	**Mechanical Properties II**
MM 31.1–31.4	Wed	17:30–18:30	H 0111	**Mechanical Properties III**
MM 32.1–32.1	Thu	9:30–10:00	H 1058	**HV Fähler**
MM 33.1–33.3	Thu	10:15–11:25	H 1058	**SYM Hydrogen in Materials: New Developments I**
MM 34.1–34.3	Thu	11:40–12:50	H 1058	**SYM Hydrogen in Materials: New Developments II**
MM 35.1–35.4	Thu	10:15–11:15	H 0107	**Phase Transitions I**
MM 36.1–36.5	Thu	11:45–13:00	H 0107	**Phase Transitions II**
MM 37.1–37.4	Thu	10:15–11:15	H 0111	**Intermetallic Phases II**
MM 38.1–38.5	Thu	11:45–13:00	H 0111	**Nanostructured Materials V**
MM 39.1–39.5	Thu	14:00–16:00	H 1058	**SYM Hydrogen in Materials: New Developments III**
MM 40.1–40.4	Thu	16:30–18:00	H 1058	**SYM Hydrogen in Materials: New Developments IV**
MM 41.1–41.19	Thu	18:00–20:00	Poster B	**Poster SYM Hydrogen in Materials: New Developments**
MM 42.1–42.6	Thu	14:00–15:30	H 0107	**Phase Transitions III**
MM 43.1–43.5	Thu	16:00–17:15	H 0107	**Phase Transitions IV**
MM 44.1–44.2	Thu	14:00–14:30	H 0111	**Bioinspired Materials**
MM 45.1–45.4	Thu	15:00–16:00	H 0111	**Nanostructured Materials VI**
MM 46.1–46.7	Thu	16:30–18:15	H 0111	**Interfaces**
MM 47.1–47.5	Fri	10:15–11:55	H 1058	**SYM Hydrogen in Materials: New Developments V**
MM 48.1–48.4	Fri	10:15–11:15	H 0107	**Phase Transitions V**
MM 49.1–49.4	Fri	11:45–12:45	H 0107	**Phase Transitions VI**

MM 50.1–50.4	Fri	10:15–11:15	H 0111	**Materials Design I**
MM 51.1–51.5	Fri	11:45–13:00	H 0111	**Materials Design II**

Symposium Hydrogen in materials: new developments
The interaction of Hydrogen with Materials as an important field of research has attracted new interest due to the greenhouse effect and the possibility to utilise hydrogen as an environment-friendly energy carrier. For mobile applications, despite major efforts a save and cost-efficient hydrogen storage system is not yet found. Nature offers two principle storage mechanisms: i) Adsorption of hydrogen molecules on surfaces (physisorption). ii) Hydrogen atoms dissolved or forming chemical compounds (chemisorption). Presently, both mechanisms are intensely investigated. Thereby novel materials are developed and their microstructure is improved by nanotechnological methods. It appears that for storage containment, distribution and handling the question of hydrogen embrittlement of structural materials is a key problem.
This Symposium will, therefore, focus on the following recent developments: (i) the interaction of hydrogen with surfaces, (ii) hydrogen interaction with microstructure, (iii) hydrogen in thin films, multi-layers, clusters and nano-powders, (iv) new light-weight, chemical and complex hydrides, and (v) hydrogen embrittlement of structural materials. The Symposium addresses both theory and experiment.
Organizers:
PD Dr. Astrid Pundt
Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen
Dr. Michael Hirscher
Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, D-70569 Stuttgart
Prof. Dr. Rüdiger Bormann
Institut für Werkstoffforschung, GKSS-Forschungszentrum Geesthacht GmbH, Max-Planck-Straße 1,D-21502 Geesthacht

Symposium Phase Transformations in Metallic Melts
Abschlusskolloquium des DFG Schwerpunktprogramms SPP1120 Phasenumwandlungen in mehrkomponentigen Schmelzen.
Organizer:
Prof. Dr. Dieter M. Herlach
Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt e.V., Linder Höhe, D-51147 Köln

Symposium Thin film magnetic materials: microstructure, reaction and magnetic coupling
With this symposium we will focus on the microstructure-properties relationship of ultra thin magnetic films utilized in state-of-the-art magnetoelectronic devices. Key questions in that respect are directed to the role of interfacial roughness and microstructural constraints due to chemical ordering and interdiffusion on magnetic, transport and tunnelling properties. Which innovative processes may be used to optimise these parameters?
Required by high storage densities or by the limited range of magnetic coupling, the typical structural scale of modern devices ranges down to a few nanometers. Therefore, these devices are destabilised by dominant interfacial contributions. How does the microstructure of such nano-scaled systems react? The symposium will highlight this field in several talks by leading experts.
Organizers:
Prof. Dr. Guido Schmitz
Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, D-48149 Münster
Prof. Dr. Andreas Hütten
Physik, Universität Bielefeld, Postfach 100 131, D-33501 Bielefeld

Symposium Modern Developments in Multiphysics Materials Simulations (SYMS)
offered jointly by the division O, HL and MM.
Thursday, February 28. For programm, see SYMS.

Symposium Ferroic materials and novel functionalities (SYNF)
offered jointly by the division MA, O, MM, DF, DS, HL, and TT
Tuesday, February 26. For programm, see SYNF.

Annual General Meeting of the Metal and Material Physics Division

Tuesday 18:00–19:00 H 0111

- Report of the chairman of the Metal and Material Physics Division.
- Invited talks and symposia for the next spring meeting 2009.
- Other topics.

MM 1: HV Adelung

Time: Monday 9:30–10:00 Location: H 1058

Invited Talk MM 1.1 Mon 9:30 H 1058

Simple ways to complex nanowires and their application — •Rainer Adelung[1], Mady Elbahri[1], Seid Jebril[1], Sebastian Wille[1], and Michael Scharnberg[2] — [1]Functional Nanomaterials, Institute for Materials Science, CAU Kiel — [2]Chair for Mulicomponent Materials, Institute for Materials Science, CAU Kiel

Many syntheses exist for nanowire fabrication. This development was driven by the promise of novel applications. In order to realize these applications, simple and rapid ways have to be found for organized nanowire fabrication, because often applications require large area coverage with nanostructures or low production costs for mass fabrication. Some contributions from our lab that were developed over the last years, ranging from tabletop chemistry to UHV processing, will be presented [1-4]. In the talk, different specific properties of nanowires will be shown and compared with bulk material; furthermore some demonstration devices for practical applications will be presented. This includes properties and applications like the electrical conductivity through metallic nanowires for sensors, or water jet reflection on nanowire surfaces for microfluidics.

[1] R. Adelung et al. Nature Mater. 3, 375, (2004) [2] M. Elbahri et al. Adv. Mater. 18, 1059 (2006) [3] M. Elbahri et al. Adv. Mater. 19, 1262 (2007) [4] C.Bain, Nature Nanotech. 2, 344 (2007)

MM 2: SYM Phase Transformations in Metallic Melts I

Time: Monday 10:15–11:15 Location: H 1058

Invited Talk MM 2.1 Mon 10:15 H 1058

Phase Formation in Multicomponent Monotectic Aluminum Alloys — Djordje Mirković, Joachim Gröbner, and •Rainer Schmid-Fetzer — Institute of Metallurgy, Clausthal University of Technology, Germany

Alloys with a miscibility gap in the liquid state are potential materials for advanced bearings in automotive and other applications. While binary alloys, such as Al-Pb or Al-Bi, are well known, the information available for ternary monotectic Al-alloys is scarce. However, the phase formation in multicomponent alloys is not only more challenging from a scientific aspect, it is also a prerequisite for a focused development of advanced alloys. This motivated our detailed study of monotectic Al-Bi-Cu-Sn alloys including both experimental and computational thermodynamic methods. Based on the initially established systematic classification of monotectic ternary Al-alloys, the first promising monotectic reaction was observed in the ternary Al-Bi-Zn system. Further ternary systems Al-Cu-Sn, Al-Bi-Sn, Al-Bi-Cu and Bi-Cu-Sn were investigated as basis for quaternary Al-Bi-Cu-Sn alloys. Experimental investigations of phase equilibria, enthalpies and solidification microstructures were combined with thermodynamic modeling. The results demonstrate that the developed precise thermodynamic description is vital to reveal the distinct multicomponent monotectic features of pertinent phase diagrams. The solidification paths of ternary monotectic alloy systems, Al-Bi-Zn, Al-Sn-Cu and Al-Bi-Cu, were also studied using thermodynamic calculations, revealing specific details of phase formation during solidification of selected alloys.

MM 2.2 Mon 10:45 H 1058

Liquid-liquid interfacial tension in multicomponent immiscible Al-based alloys — •Walter Hoyer[1] and Ivan Kaban[2] — [1]Technische Universität Chemnitz, Institut für Physik, 09107 Chemnitz — [2]Technische Universität Chemnitz, Institut für Physik, 09107 Chemnitz

Liquid-liquid interfacial tension and density difference of the coexisting phases have been determined in wide temperature and composition ranges in binary Al-Bi, ternary Al-Bi-Cu, Al-Bi-Si, Al-Bi-Sn and quaternary Al-Bi-Cu-Sn alloys.

It is found that the interfacial tension between Al-rich and Bi-rich liquid phases increases when either Cu or Si is added and it decreases when Sn is added. Simultaneous addition of Cu and Sn in equal quantity results in a decrease of the interfacial tension at low temperature and in its increase at high temperature. Temperature dependences of the interfacial tension in all alloys studied are well described by the function $\sigma_{\alpha\beta} = \sigma_0(1 - \mathcal{T}/\mathcal{T}_C)^\mu$ with a constant σ_0 and the critical point exponent $\mu = 1.3$.

MM 2.3 Mon 11:00 H 1058

Gefügemorphologien gerichtet erstarrter monotektischer Legierungen — Martin Seifert und •Lorenz Ratke — Institut für Materialphysik im Weltraum, DLR, Cologne, Germany

Bei der gerichteten Erstarrung von Legierungen mit exakt monotektischer Zusammensetzung werden abhängig von der Erstarrungsgeschwindigkeit v und dem Temperaturgradienten G an der monotektischen Reaktionsfront verschiedene Morphologien beobachtet. Fasern bei hohen Gradienten und kleinen Geschwindigkeiten, perlschnurartige Gebilde bei mittleren Gradienten und größeren Erstarrungsgeschwindigkeiten. Bei kleinen Temperaturgradienten treten immer irreguläre Tropfenanordnungen auf. Die Mechanismen der Bildung der verschiedenen Gefügemorphologien sind nicht verstanden. Der Vortrag präsentiert Experimente an den Systemen Al-In, Al-Bi, Al-Pb bei denen systematisch v in Bereichen von 0,5 μm bis 5 μm und G im Bereich von 3 bis 8 K/mm variiert wurden. Die verschiedenen Gefügetypen werden charakterisiert und ihre Entstehung im Rahmen neuerer Theorien zum konvektionsbeeinflussten Wachstum an der monotektischen Front diskutiert.

MM 3: SYM Phase Transformations in Metallic Melts II

Time: Monday 11:45–12:30 Location: H 1058

MM 3.1 Mon 11:45 H 1058

Thermophysical Properties of Liquid Ternary Metallic Alloys — Ivan Egry and •Jürgen Brillo — Institut für Materialphysik im Weltraum, DLR, 51170 Köln

Thermophysical properties of liquid metals are difficult to measure, but highly relevant, both from an application and a fundamental point of view. On one hand, they are required for quantitative modelling of industrial processes such as solidification and welding; on the other, they are sensitive indicators of ordering phenomena in the liquid phase. In binary and multicomponent alloys, the so called excess quantities are of particular interest. They describe the deviation of thermodynamic and thermophysical properties from the respective ideal mixing laws. In this project we have determined surface tensions and densities of the two ternary systems Cu-Fe-Ni and Ag-Al-Cu over the entire concentration range, including the limiting binary systems. The measurements have been performed on electromagnetically levitated liquid drops using non-contact diagnostic tools, like the oscillating drop technique for surface tension and a shadowgraph technique for density measurements. A wide temperature range, including the undercooled regime, was covered by the experiments. Surface tension data were modelled by the Butler equation using available Gibbs excess free energies, and generally good agreement was found. From the density data, the excess volumes were calculated. They constitute a non negligible contribution and can have either sign.

MM 3.2 Mon 12:00 H 1058

Messungen der fest-flüssig Grenzflächenenergien in ternären

Systemen — Annemarie Bulla[1], Carlos Carreno-Bodensiek[2], •Emir Subasic[1], Ralf Berger[1], Andreas Bührig-Polaczek[1] und Andreas Ludwig[3] — [1]Gießerei-Institut der RWTH Aachen, 52072 Aachen, Deutschland — [2]Department of Electromechanical Engineering, Faculty of Duitama, Duitama, Columbia — [3]Department Metallurgie, Montanuniversität Leoben, 8700 Leoben, Österreich

Die fest-flüssig Grenzflächenenergie spielt während des Erstarrungsprozesses für die Keimbildung und das Wachstum der Phasen eine zentrale Rolle. Sie geht als wichtiger Parameter in viele analytische und numerische Erstarrungs- und Reifungsmodelle ein. In der Literatur finden sich nur sehr begrenzt experimentell bestimmte Werte. Für ternäre und höherkomponentige Systeme existieren bisher keine Messungen. Die zentrale Zielsetzung der vorliegenden Arbeit bestand darin, eine geeignete Vorrichtung für die Messung der fest-flüssig Grenzflächenenergie aufzubauen und auf im Rahmen des Schwerpunktprogrammes relevante ternäre Legierungssysteme anzuwenden. Dazu wurde entsprechend den Arbeiten der Gruppe von Prof. J.D. Hunt in Oxford eine radiale Wärmeflussapparatur aufgebaut, die die Einstellung eines sehr stabilen radialen Temperaturgradienten erlaubt, indem eine zylindrische Probe entlang ihrer Achse geheizt und auf der Außenseite gekühlt wird. Durch Formanalyse von Gleichgewichtskorngrenzenfurchen und die numerische Bestimmung der lokalen Unterkühlung entlang der Korngrenzenfurchung wurde der Gibbs-Thomson-Koeffizient und daraus die fest-flüssig Grenzflächenenergie bestimmt.

MM 3.3 Mon 12:15 H 1058

Phase Equilibria of Nanoscaled Systems — •Gerhard Wilde[1], Harald Rösner[2], Peter Bunzel[2,3], and Jörg Weissmüller[2,3] — [1]Universität Münster, Institut für Materialphysik — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie — [3]Technische Physik, Universität des Saarlandes

The impact of the morphology of the interface of matrix-encased nanoparticles on the melting transition has been investigated. To elucidate the interface contribution clearly, material of identical chemical composition has been synthesized by different processing pathways, resulting in distinctly different interface topologies. These results are discussed with respect of the mechanisms that lead to a size dependence of the melting temperature. Aside from the particle/matrix interfaces, internal heterophase interfaces necessarily occur, if multicomponent and especially multiphase materials are addressed. In multicomponent and nanoscaled alloy systems, interface segregation and interface-induced stresses are known to affect the phase boundary lines of the equilibrium phase diagrams at fixed size. Yet, already the presence of internal heterophase interfaces contributing an excess free energy is sufficient to severely modify the phase equilibrium and the associated phase transformations in nanosize alloy systems. Here, results on the constitutive behavior of binary nanoscaled model alloys obtained by modeling will be highlighted. In addition, experimental results concerning the constitutive behavior of nanoscale alloy systems and concerning a new approach for obtaining nanoscale systems with well-defined size are presented. Support by the DFG is gratefully acknowledged.

MM 4: Nanostructured Materials I

Time: Monday 10:15–11:30 Location: H 0107

MM 4.1 Mon 10:15 H 0107

Electrochemically induced surface charge effect on the properties of nanoporous Au-Fe alloys — •Ajay Kumar Mishra[1], Chandrahas Bansal[1,2], and Horst Hahn[1] — [1]Institute for Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe 76021, Germany — [2]School of Physics, University of Hyderabad, Hyderabad 500 046, India

Nanoporous Au-Fe alloys consisting of nanoparticles of about 5 nm diameter were synthesized by inert gas phase condensation. Charge was induced electrochemically on the surface of the nanoparticles, and in-situ measurements of strain, magnetization, and conductivity were carried out during the charging and decharging process taking place in the electrochemical cell. The observed strain could be explained to arise from a Coulomb pressure produced by the surface charge on the metal. The variation of magnetization with charging was also found to be consistent with the effect of this pressure. A charge induced variation in the dc electrical conductivity of about 6 percent was observed. An explanation of the rate of change of conductivity with charge was provided in terms of the additional charge density produced by the induced charge. Similarly at the microscopic level, Mossbauer isomer shift and quadrupole splitting were measured and showed a small but reversible behaviour with charge.

MM 4.2 Mon 10:30 H 0107

Charge induced ITO transistor for printable electronics — •Subho Dasgupta, Sebastian Gottschalk, Robert Kruk, and Horst Hahn — 1Institute of Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany

Although research on printable electronics has received increasing attention in the past two decades there are essential scientific and technical problems still to be addressed prior to commercialization. In general, printable electronics with organic or inorganic channels suffer from either very low mobility (pentacene or amorphous silicon FETs) or their fabrication is complicated, costly, requires sophisticated techniques, or involves high processing temperature (polycrystalline silicon or semiconducting oxide FETs). We have fabricated an alternative electrochemically gated JFET with commercial ITO nanoparticles as a channel (with nearly metallic conductance) and an electrolyte as a gate. The device principle is based on a charge induced variation of drain current without any redox reaction at the electrolyte/particle interface. Depending on the electrolyte used, the on/off ratio can be as high as 103. The calculated field-effect mobility is in the range 30-60 cm^2/Vs when the whole channel is considered as an array of nanowires whose diameter is equal to the average neck diameter of the nanoparticles. The subthreshold swing (415 mVdec-1) is lower than most of the printable FETs reported so far. The high conductance of the channel can offer added advantage with high on-state current for submicron device sizes. Similar devices fabricated with a solid polymeric electrolyte as a gate dielectric can be ultracheap and readily printable.

MM 4.3 Mon 10:45 H 0107

Energy Transfer in Solution-Based Complexes of CdTe Nanocrystals Electrostatically Bound by Calcium Ions — •Sergiy Mayilo, Jan Hilhorst, Andrei S. Susha, Cornelia Höhl, Thomas A. Klar, Andrey L. Rogach, and Jochen Feldmann — Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians Universität München, Germany

Colloidal semiconductor nanocrystals with controllable surface properties are attractive objects for use as building blocks in different functional structures within the bottom-up assembly approach. We produced stable complexes from differently-sized water soluble CdTe nanocrystals capped by mercaptoacid stabilizers through electrostatic interactions of negatively charged carboxylic groups of capping ligands with positively charged Ca(II) cations. Energy transfer between smaller nanocrystals (donors) and larger nanocrystals (acceptors) in fabricated complexes is demonstrated by means of steady-state and time-resolved photoluminescence spectroscopy, paving the way to nanocrystal-based light harvesting structures.

MM 4.4 Mon 11:00 H 0107

Electronic transport properties of individual chemically reduced graphene oxide sheets — •cristina gómez-navarro[1], thomas weitz[1], alexander bittner[1], mateo scolari[2], alf mews[2], marko burghard[1], and klaus kern[1] — [1]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Chemistry, University of Siegen, D-57068 Siegen, Germany

The peculiar electronic properties of graphene sheets have attracted substantial interest in the scientific community during the past few years (1-2). Micromechanical cleavage is currently the most effective method to produce high-quality graphene sheets. However this method does not enable the large-scale production required for most applications. Consequently alternative production methods for graphene sheets are highly desirable. Here we report on the electronic transport properties of single graphene sheets obtained via chemical reduction of graphite oxide. We find that reduced single layers exhibit room

temperature conductivities of 0,05-2 S/cm and field effect mobilities of 2-200cm2/Vs. Temperature dependent electrical measurements and Raman spectroscopic investigations reveal that charge transport occurs via variable range hopping between intact graphene islands with sizes of the order of several nanometers. The electrical properties of sheets composed of two and more layers will be also discussed (3).

1. K. S. Novoselov et al., Science 306, 666 (2004).
2. C. Berger et al., Science 312, 1191 (2006).
3. C.Gómez-Navarro et al. Nanoletters (2007)

MM 4.5 Mon 11:15 H 0107

Observation of coherent electron motion in disordered granular metals — •Michael Huth, Dirk Klingenberger, and Christina Grimm — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany

We observed a $\sigma \propto \sqrt{T}$-dependence of the electrical conductivity σ vs. temperature T in metal-insulator nanocomposite samples prepared by electron beam induced deposition. This dependence was recently predicted as a low-energy contribution in the metallic regime of 3D granular metals if electron-electron interactions are taken into account[1]. It is the consequence of the occurence of a large-scale coherent electron motion and signifies a universal resistive behavior in granular metals even in the presence of disorder.

[1]I. S. Beloborodov, K. B. Efetov, A. V. Lopatin, and V. M. Vinokur, Phys. Rev. Lett. **91**, 246801 (2003); I. S. Beloborodov, A. V. Lopatin, V. M. Vinokur, and K. B. Efetov, Rev. Mod. Phys. **79**, 469 (2007)

MM 5: Nanostructured Materials II

Time: Monday 12:00–13:00 Location: H 0107

MM 5.1 Mon 12:00 H 0107

Laser-induced nanotube-nanotube interactions — •Jessica Walkenhorst[1], Martin E. Garcia[1], and Harald O. Jeschke[2] — [1]Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [2]Institut für theoretische Physik, Universität Frankfurt, Robert-Mayer-Str. 8-10, 60054 Frankfurt, Germany

We have investigated the possibility of achieving welding of two single wall nanotubes by making use of topological defects and femtosecond laser excitation. Based on molecular dynamics simulations performed on time-dependent potential energy surfaces, and considering explicitly the shape, energy and duration of the laser pulse, we describe the ultrafast dynamics of two defective nanotubes in contact to each other immediately after femtosecond excitation. We discuss the role of different defects and their respective behaviour under laser heating.

MM 5.2 Mon 12:15 H 0107

Breaking transition of carbon nanotubes and graphene under stress — •Juergen Dietel and Hagen Kleinert — Institut fuer Theoretische Physik, Freie Universitaet Berlin

We calculate the breaking transition of carbon nanotubes and graphene under homogeneous external stress as a function of temperature.

MM 5.3 Mon 12:30 H 0107

Modeling of Surface Modification and Nanostructuring on Metals due to a Femtosecond Laser Pulse — •Dmitriy Ivanov[1], Baerbel Rethfeld[1], Gerard O'Connor[2], Thomas Glynn[2], Zhibin Lin[3], and Leonid Zhigilei[3] — [1]Physics Department, Technical University of Kaiserslautern, Kaiserslautern, Germany — [2]National Centre for Laser Applications, National University of Ireland Galway, Galway, Ireland — [3]Materials Science Department, Univeristy of Virginia, Charlottesville, USA

The atomistic-continuum approach to study nanostructuring processes on metals due to fast laser energy deposition is presented. The intense, short-pulsed laser interactions are involving mechanical, thermal, and phase perturbations. Many of those non-equilibrium processes are impossible to study experimentally and difficult to model at all levels: ab-initio, atomistic, and continuum. We address this challenge combining the advantages of different approaches. Namely, the kinetics of fast non equilibrium phase transformations is treated at atomic level; and free carrier dynamics (fast electron heat conduction and laser-induced electron-phonon nonequilibrium)is accounted for in continuum part.

The combined model was applied to study the formation of nanojets on thin Ni films in femtosecond laser pulse experiments. The calculations show that surface nanostructuring is due to the interplay of three processes: establishment of temperature gradient in radial directions causes the elasto-plastic deformations; relaxation of laser-induced pressure leads to the ejection of melted material; fast electron heat conduction in 3D effectively cools down and freezes the ejected matter.

MM 5.4 Mon 12:45 H 0107

Molecular Dynamics Simulations of Nanoglasses — •Daniel Sopu[1], Karsten Albe[1], and Herberg Gleiter[2] — [1]Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt — [2]Inst. f. Nanotechnologie, FZ Karlsruhe, D-76021 Karlsruhe

We present molecular dynamics simulations on the structure and stability of nanoglasses that can be generated by consolidating nanometer-sized glassy spheres at high pressures (several GPa). Our results suggest that nanoglasses consist in the as prepared state of glassy regions resulting from the consolidated spheres and interfaces between these glassy regions. In these glass/glass interfaces, the free volume is enhanced and the nearest neighbor co-ordinations deviate from the ones in the glassy regions. If these nanoglasses are annealed, the enhanced free volume in the glass/glass interfaces delocalize and, thus, modifies the atomic structure of the entire material. In conclusion, nanoglasses may pave the way to tune the free volume (density) of glasses at constant chemical composition.

MM 6: Diffusion I

Time: Monday 10:15–11:30 Location: H 0111

MM 6.1 Mon 10:15 H 0111

Fast ionic mobility in cryolite studied by quasielastic neutron scattering — •Sandro Jahn[1], Jacques Ollivier[2], and Franz Demmel[3] — [1]GeoForschungsZentrum Potsdam, Telegrafenberg, 14473 Potsdam — [2]Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France — [3]ISIS Facility, Chilton, OX11 0QX, UK

The relation between ionic mobility and conductivity at high temperature of the perovskite fluoride cryolite, Na_3AlF_6, is studied by quasielastic neutron scattering (QENS). Up to $T = 880$ °C the conductivity is dominated by jump diffusion of Na ions. At higher temperatures, a considerable broadening of the QENS spectra and the development of a liquid-like diffraction peak is observed. In the temperature range between $T = 880$ °C and the melting point ($T_m = 1013$ °C), the presence of about one percent of partial melt, that is expected from the phase diagram, causes a high mobility of almost all F ions of the system. The Q-dependence of the line width suggests a set-in of translational diffusion of fluorines at this temperature. This additional degree of translational movements could reason the jump-like increase in the ionic conductivity observed macroscopically.

MM 6.2 Mon 10:30 H 0111

Atomistic simulation of grazing incidence diffuse x-ray scattering from point defects — •Ruslan Kurta, Vladimir Bugaev, Melissa Delheusy, Andreas Stierle, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Heisenbergstr.3, D-70569 Stuttgart, Germany

The investigation of defects in the vicinity of surfaces and interfaces is a current challenge, because such defects control important phe-

nomena in the subsurface region, such as chemical reactions, ion conduction, performance of superconducting cavities. The challenge here is to understand microscopically the coupling of the defect-induced strain field to the interfaces. The goal of our project is the x-ray study and theoretical modeling of the strain field of point defects close to interfaces. Here, in particular, we present the results of an investigation of dissolved interstitial oxygen in the subsurface region of Nb (110), which plays a key role in the performance of high frequency cavities. The x-ray data were obtained from the diffuse x-ray scattering experiments under glancing-angle conditions. We use a semiphenomenological Kanzaki-Krivoglaz approach to calculate the strain field around the point defect. For modeling of the diffuse x-ray scattering distribution in the vicinity of a surface we use a fully atomistic real-space "large-sphere" method. This allows one to obtain quantitative information about the defect distribution close to a surface. On the basis of the depth-resolved x-ray data we determined the subsurface concentration profile of the dissolved oxygen.

MM 6.3 Mon 10:45 H 0111

Frühe Ausscheidungsstadien in Al-Cu-Mg-Legierungen – EXAFS/XANES Messungen an der Cu k-Kante — •Torsten E.M. Staab[1], Benedikt Klobes[1] und Esther Dudzik[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, D-53115 Bonn, Germany — [2]Hahn-Meitner-Institut Berlin/Bessy, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

Größe und Verteilung nanoskaliger Cluster — sogenannter Guinier-Preston- (GP) oder Guinier-Preston-Bagaryatsky-Zonen (GPB) — bestimmen die Festigkeit von Aluminiumlegierungen. Diese Cluster behindern die Bewegung von Versetzungen. Al-Legierungen für den Flugzeugbau (AA2024) enthalten Kupfer und Magnesium als Hauptlegierungsbestandteile. EXAFS/XANES-Messungen an der Cu k-Kante zeigen, dass sich die atomare Umgebung der Cu-Atome schon während der ersten Stunden bei Raumtemperatur-Lagerung ändert. Durch den Vergleich mit ab-initio Rechnungen können wir die Änderungen der Spektren der Bildung von Cu-Mg-Clustern (GPB-Zonen) zuordnen. Während des weiteren Alterungsprozesses der Legierung ändert sich die chemische Zusammensetzung und die Gitterstruktur der Ausscheidungen hin zur stabilen S-Phase (Al_2CuMg), was sich in der lokalen atomaren Umgebung des Legierungselementes Kupfer widerspiegelt.

MM 6.4 Mon 11:00 H 0111

Frühstadien der Ausscheidungsbildung in Al-Mg-Cu-Legierungen - Simulationsrechnungen zu Positronenannihilationssignalen — •Björn Korff und Torsten Staab — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn, Germany

Nach Abschrecken lösungsgeglühter Al-Mg-Cu-Legierungen (AA 2024) bilden sich schon bei Raumtemperatur Ausscheidungen. Diese Agglomerate weniger Atome werden als Frühstadien bezeichnet. Sie erreichen nach einer Auslagerung von fünf Tagen bei Raumtemperatur eine Größe von 1-2 nm und sind für die Härte des Materials verantwortlich. Die Struktur dieser frühen Ausscheidungen ist im Gegensatz zur Gleichgewichtsphase, die erst bei höheren Temperaturen erreicht wird, noch nicht endgültig geklärt.

Zur Untersuchung der Ausscheidungsbildung wurden in Simulationsrechnungen die Positronenannihilationsparameter für verschieden Atomkonfigurationen berechnet. Ein Vergleich mit Positronen-Messung an den Legierungen gibt dann Hinweise über die Struktur der Ausscheidung. Die Atomkoordinaten der getesteten Stukturen wurden mit Hilfe des ab-initio Codes SIESTA relaxiert. Die Methode der Positronenannihilation ist besonders empfindlich für Leerstellen, in denen die Positronen stark lokalisiert werden. So erhält man Informationen über den Entstehungsprozess der Ausscheidungen, da die Diffusion der Fremdatome bei Raumtemperatur über eingeschreckte Leerstellen vermittelt wird.

MM 6.5 Mon 11:15 H 0111

Early stages of precipitation in AlMgSi alloys: an investigation by positron annihilation — •Benedikt Klobes, Torsten E. M. Staab, Matz Haaks, and Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, D-53115 Bonn

Aluminium alloys on the basis of AlMgSi, the so-called 6000 series, are commonly used in a wide range of industrial applications due to their good mechanical properties as well as their weldability. These properties are induced by the precipitation of nanoscaled agglomerates of Mg and Si atoms which are formed during specific heat treatments. Although these alloys have been the object of intense investigations, it has been impossible to reveal the atomic structures of these precipitates up to now. Thus, the understanding of the precipitation sequence remains incomplete. Measuring the positron lifetime and the Doppler broadening of the annihilation radiation directly after solution heat treatment and quenching we recently observed a significant change of the mean positron lifetime as well as the momentum distribution during subsequent storage at room temperature. The first stages of precipitation could be investigated in both high purity alloys and a commercial alloy AA6013 this way. With these results we hope to throw a little light on the controversially discussed precipitation sequence of AlMgSi alloys.

MM 7: Diffusion II

Time: Monday 12:00–13:00 Location: H 0111

MM 7.1 Mon 12:00 H 0111

Adaptive jump barrier height in Monte Carlo configuration kinetics. — •Martin Leitner[1], Doris Vogtenhuber[2], Wolfgang Pfeiler[1], and Wolfgang Püschl[1] — [1]Dynamics of Condensed Systems, Faculty of Physics, University of Vienna, Strudlhofgasse 4, A-1090 Wien — [2]Computational Materials Science, Faculty of Physics, University of Vienna, Sensengasse 8, A-1090 Wien

In usual MC simulations of configuration kinetics atom jump probabilities are calculated from energies of the initial and/or final bound states of the moving atom, leaving aside the exact energy of the intermediate saddle point state. This energy may however be critically influenced by the local atomic environment. We propose a strategy to explicitly take account of this influence. The basis is ab initio calculation of representative jump paths in the framework of the nudged elastic band method. From these results, an influence function is derived which modifies the energy of the saddle point and therefore the effective jump barrier height as calculated from the initial and final states according to a cluster expansion scheme. The overall effect is demonstrated on the NiAl system.

MM 7.2 Mon 12:15 H 0111

Frühstadien der Ausscheidungsbildung in AlCu-, AlMgCu-Legierungen : Ab-initio Rechnungen zu Leerstellenbildungsenthalpien — •Iris Kohlbach und Torsten Staab — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn

Durch die Ausscheidung von Fremdphasen kommt es bei Aluminiumlegierungen zur Aushärtung. Während die Ausscheidungssequenz von AlCu-Legierungen sehr gut bekannt ist, liegen die Frühstadien der AlMgCu-Legierungen dagegen noch nahezu gänzlich im Bereich der Spekulation. Zur Untersuchung der Rolle von Leerstellen beim Ausscheidungsprozess im AlCu wurden die Bildungsenthalpien für Leerstellen auf den verschiedenen Untergittern von Al_2Cu (Θ'- und Θ-Phase) mit Hilfe des ab-initio-Codes SIESTA bestimmt. Für Al_2MgCu wurden diese für die S''- und S-Phase berechnet, wobei aus den zahlreichen Vorschlägen zur S''-Phase die Vorschläge von Cuisat bzw. Wolverton [1] ausgewählt wurden. Unsere Ergebnisse zu Leerstellenbildungsenthalpien für AlCu-Phasen zeigen z.B. deutlich, dass sich hier keine Leerstellenagglomerate bilden. SIESTA liefert neben den Gesamtenergien eines Systems zusätzlich relaxierte Atompositionen, die für den Vergleich mit experimentellen Daten von großer Wichtigkeit sind.

[1] Wang/Starink, Int Mater Rev., 2005, Vol. 50, pp 193-215

MM 7.3 Mon 12:30 H 0111

Steady drift-diffusion model of impurity induced subcritical crack propagation — •Mario Koch[1] and Peter Streitenberger[2] — [1]Institut der Feuerwehr Sachsen-Anhalt, Biederitzer Str. 5, 39175 Heyrothsberge, Deutschland — [2]Otto-von-Guericke-Universität Magdeburg, PSF 4120, 39016 Magdeburg, Deutschland

The stress-driven diffusion of point defects to a slowly moving crack

under mixed-mode loading is studied by solving the corresponding drift-diffusion equation in a co-moving reference system. Numerical solutions for the quasi-stationary concentration fields and flow field patterns are presented, which reveal important insights into the point-defect migration kinetics near a steadily advancing crack. In particular, it is shown that only impurities within a limited drift-diffusion zone, of which the extension depends on the average crack growth rate, are able to migrate to the crack tip. Considering the existence of a critical impurity concentration per crack length advance as the basic criterion for failure of the material, the crack growth behaviour in form of the crack growth rate versus stress intensity factor curve is calculated. In the case where the size of the plastic zone is very small in comparison with the drift-diffusion zone stage I crack growth is observed, if the size of the plastic zone is very large in comparison with the drift-diffusion zone stage II crack growth is observed.

MM 7.4 Mon 12:45 H 0111

Re-orientation behaviour of c-variant FePt thin films — •Marcus Rennhofer[1], Miroslav Kozlowski[2], Bart Laenens[3], Bogdan Sepiol[1], Rafal Kozubski[2], Andre Vantomme[3], Johan Meersschaut[3], and Gero Vogl[1] — [1]University of Vienna, Vienna, Austria — [2]Jagiellonian University Cracow, Cracow, Poland — [3]Instituut for Kern- en Stralingsfysika

The magnetocrystalline and thermal stability of $L1_0$-FePt makes this alloy suitable for ultrahigh density recording. Various experiments with bulk $L1_0$-FePt dealing with diffusion and ordering dynamics have been performed [1, 2].

Our Monte Carlo (MC) simulations show that the c-variant of the $L1_0$ superstructure (easy axis of the magnetisation out of plane of the thin film samples) is unstable. The monoatomic planes re-orient creating a-domains (easy axis of the magnetic field in the film plane). Our recent conversion electron Mössbauer spectroscopy (CEMS) experiments on -variant ^{57}FePt(50 nm)/MgO(001) thin films show evidence of this re-orientation behaviour. The picture arising from our results is as follows: an re-orientation takes place but reverts after a certain time and then saturates. The effect depends on the annealing temperature. An additional capping of the films suppresses the effect almost completely.

[1] M. Rennhofer et al. Phys. Rev. B. 74(10), 104301 (2006).
[2] R. Kozubski et al J. of Phase Equil. and Diff. 26(5), 482 – 486 (2005).

MM 8: HV Mücklich

Time: Monday 14:00–14:30 Location: H 1058

Invited Talk MM 8.1 Mon 14:00 H 1058

Microstructure tomography - an essential tool to understand 3D microstructure and local degradation effects — •Frank Muecklich — Universität des Saarlandes, Saarbruecken, Germany

Since the traditional 2D planar section sampling in cases of complex shaped microstructures often supplies insufficient information, the quantitative investigations of the essential correlations between processing, microstructure and properties in advanced materials call for an adequate imaging and quantification of the 3D microstructure. X-ray and electron tomography still suffer from a lack of resolution or field of view size respectively. Representative characterization can be done by the help of microstructure tomography [1]. This method combines the excellent target preparation possibilities of a focused ion beam (FIB) with all types of SEM contrast. It enables extensive serial sectioning of representative sample volumes and the imaging of chemical and structural phenomena with a resolution of about 2-10nm. Once the 3D data set is available, their exploitation in 3D image analysis provide quantitative insights into the relation between processing, structure and properties. So far the complex formation of multiphase 3D microstructures, the related interface as well as seeding phenomena and also very local degradation effects were investigated. The talk will provide a general overview of the potential and the limits of this technique supported by examples of some technical relevance in different materials. [1] Lasagni, Marks, Holzapfel, Degischer and Muecklich: Acta Materialia 55(2007)3875-3882

MM 9: SYM Phase Transformations in Metallic Melts III

Time: Monday 14:45–16:00 Location: H 1058

Invited Talk MM 9.1 Mon 14:45 H 1058

Atomic Diffusion in Liquid Alloys — •Andreas Meyer[1,2], Suresh Mavila Chathoth[2], Winfried Petry[2,3], Tobias Unruh[3], and Marek Koza[4] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Physik Department E13, TU München — [3]FRM-II, TU München — [4]Institut Laue Langevin, Grenoble

We investigate the atomic motion in liquids on Ni-, Pd-, and Zr- basis in order to clarify the microscopic transport mechanisms. High-resolution energy and momentum information from neutron scattering experiments allows to study how the atomic dynamics depends on structural properties, and in some special cases to derive the self diffusion coefficient of one particular component on an absolute scale. Results on binary alloys and multicomponent bulk glass forming melts, reveal non-trivial mechanisms of mass transport. We show that the relation between equilibrium melt structure and atomic transport is well described by a mode-coupling theory. Our findings are discussed in the context of results obtained by molecular dynamics simulations and long capillary diffusion experiments performed by other groups within the SPP 1120.

MM 9.2 Mon 15:15 H 1058

Influence of thermodynamic forces on diffusion in metallic melts measured by ex-situ and in-situ capillary techniques — •Axel Griesche[1,2], Michael-Peter Macht[2], and Günter Frohberg[3] — [1]Institut für Materialphysik im Weltraum, DLR, Linder Höhe, 51170 Cologne — [2]Dept. Materials, Hahn-Meitner-Institute Berlin, Glienicker Str. 100, 14109 Berlin — [3]Institute of Material Sciences and Technology, Technical University Berlin, Hardenbergstr. 36, 10623 Berlin

The Darken relation that correlates interdiffusion coefficients, self diffusion coefficients and thermodynamic factors was studied in different metallic melts. Interdiffusion and self diffusion in $Al_{80}Ni_{20}$, $Al_{77}Ni_{20}Ce_3$ and $Pd_{40}Cu_{15}Ni_{25}P_{20}$ melts have been measured above the liquidus temperature using classical capillary methods and a novel X-ray radiography method. The chemical diffusion profiles of the ex-situ technique were determined by means of EDS whereas for the in-situ technique the profiles were determined from absorption pictures. Self diffusion coefficients were determined from penetration profiles of stable enriched ^{62}Ni, ^{142}Ce, ^{108}Pd, and ^{65}Cu isotopes measured by ICP-MS and for Ni additionally by QNS. The thermodynamic factors of Al-based alloys were calculated from chemical potential data whereas the thermodynamic factor of Pd-alloys was estimated from partial mixing enthalpies. In liquid Al alloys the enhancement of chemical diffusion with respect to self diffusion correlates linearly with the thermodynamic factor. For Pd alloys the experimental findings are discussed only qualitatively.

MM 9.3 Mon 15:30 H 1058

Molecular dynamics computer simulation of crystal growth and melting in $Al_{50}Ni_{50}$ — Ali Kerrache[1], •Juergen Horbach[1,2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, 51147 Köln

The melting and crystallization of $Al_{50}Ni_{50}$ are studied by means of molecular dynamics computer simulation, using a potential of the em-

bedded atom type to model the interactions between the particles. Systems in a slab geometry are simulated where the B2 phase of AlNi in the middle of an elongated simulation box is separated by two planar interfaces from the liquid phase, thereby considering different crystal orientations (100, 110, and 111). By determining the temperature dependence of the interface velocity, an accurate estimate of the melting temperature is provided. For the different orientations similar values around 0.002 m/s/K are found for the kinetic coefficient. This value is about two orders of magnitude smaller than that found for one-component systems. We discuss this finding in the framework of the Wilson-Frenkel model, considering also structure and diffusion dynamics in the vicinity of the liquid-crystal interface.

MM 9.4 Mon 15:45 H 1058

Entropy in Molecular Dynamics simulated AlyNi40-yZr60 melts. — •Helmar Teichler and Mohammed Guerdane — Inst. f. Materialphysik, Universität Göttingen, Göttingen, Germany

Entropy plays a major role in stabilizing melts against crystallization, and entropy (and enthalpy) release are the main phenomena that determine solidification. Despite its importance, little is known at present about the microscopic origin of entropy in melts, especially for complex multi-component metallic systems with steric and chemical short range order. Regarding this, exploiting ergodicity, we present here results from isothermal molecular dynamics simulations for the entropy in the pseudo binary AlyNi40-yZr60 series (y=0 - 40 at% Al), combining thermal integration along the temperature axis and Kirkwoods (1935) coupling parameter approach. In the simulations the AlNiZr model of Guerdane and Teichler (PRE 65, 014203 (2001)) is used.

We show in particular that our method provides entropy data with an internal reliability better than 0.01 kB. In the AlyNi40-yZr60 series, we find a slightly negative total entropy of mixing. The configuration entropy of the (trigonal prismatic) Ni40Zr60 melt at 2400 K turns out below that of liquid Zr while the configuration entropy of (binary polytetrahdral) Al40Zr60 melt lies above. These observations and the temperature dependence of the phenomena shall be discussed.

MM 10: SYM Phase Transformations in Metallic Melts IV

Time: Monday 16:30–18:00 Location: H 1058

MM 10.1 Mon 16:30 H 1058

Quasielastic Neutron Scattering on Refractory Al-Ni melts — •Sebastian Stüber[1], Andreas Meyer[2], Dirk Holland-Moritz[2], Helena Hartmann[2], and Tobias Unruh[3] — [1]Physik Department E13, Technische Universität München, 85747 Garching — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR) 51170 Köln — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, 85747 Garching

In this talk we will present results of quasielastic neutron scattering at the time of flight spectrometer Tof-Tof of the FRM II used to study atomic dynamics in melts of binary Al-Ni alloys that are the basis of a large variety of high temperature applications. In order to undercool the melts deeply below the melting temperature and to avoid reactions with crucible materials, the liquids are containerlessly processed under high purity conditions by application of the electromagnetic levitation technique. Due to the containerless processing the measured dynamic structure factors are not affected by scattering from a sample container such that the quasielastic neutron scattering measurements were possible also at large momentum transfer. From the measured dynamic structure factors Ni self-diffusion coefficients are determined as a function of alloy composition and temperature. At constant temperature, the Ni self diffusivity is constant within a wide compositional range.

MM 10.2 Mon 16:45 H 1058

Structure and dynamics of liquid $Ni_{36}Zr_{64}$ — •Dirk Holland-Moritz[1], Oliver Heinen[1], Andreas Meyer[1], Sebastian Stüber[2], Thomas Voigtmann[1], Tobias Unruh[3], and Thomas Hansen[4] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Physik Department E13, Technische Universität München, 85747 Garching, Germany — [3]Forschungsneutronenquelle Heinz Maier Leibnitz (FRM II), Technische Universität München, 85747 Garching, Germany — [4]Institut Laue-Langevin, 38042 Grenoble, France

We investigated the atomic dynamics and the static structure factor of $Ni_{36}Zr_{64}$ melts. To undercool the liquids below the melting temperature and to avoid reactions with crucible materials, the melts are containerlessly processed under high purity conditions by electromagnetic levitation. This technique is combined with quasielastic neutron scattering at the time of flight spectrometer TOFTOF of the FRM II and with elastic neutron scattering at the diffractometer D20 of the ILL. Partial static structure factors have been derived via isotopic substitution. From the quasielastic neutron scattering studies the Ni self-diffusivity is determined. The partial static structure factors indicate a chemical short-range order in liquid $Ni_{36}Zr_{64}$ and a topological short-range order that is different from the icosahedral short-range order found in most other metallic melts. The experimental results are discussed in the framework of mode coupling theory. We thank Deutsche Forschungsgemeinschaft for funding within the priority programme 1120 under contract Nos. HO1942/6-3 and ME1958/2-3.

MM 10.3 Mon 17:00 H 1058

Computational optimisation of multi-component hard sphere liquids — •Helmut Hermann[1], Antje Elsner[1], Valentin Kokotin[1], Kristin Lochmann[2], and Dietrich Stoyan[2] — [1]Institute for Solid State and Materials Research, IFW Dresden, P.O.Box 270116, D-01171 Dresden, Germany — [2]Freiberg University of Mining and Technology, Institute of Stochastics, Agricolastr. 1, D-09596 Freiberg, Germany

The atomistic simulation of multi-component metallic melts is a difficult task since there are no realistic interaction potentials for systems consisting of more than three species. Therefore, the generalised Bernal's model for liquids is used as an approach to the structure of multi-component liquid and amorphous metallic alloys. Varying size distribution and chemical composition, parameter ranges are determined leading to maximum values of the mean packing fraction. This generalised Bernal's model is combined with Miedema's macroscopic atom model for predicting enthalpy effects in alloys. The results of the simulations correspond at least qualitatively to empirical rules of high glass forming ability of multi-component metallic melts.

MM 10.4 Mon 17:15 H 1058

Crystal nucleation in colloidal model systems - Is Classical Nucleation Theory still state of the art? — •Hans Joachim Schöpe[1], Gary Bryant[2], and William van Megen[2] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland — [2]Department of Applied Physics, Royal Melbourne Institute of Technology, GPO Box 2476V, Melbourne 3001, Australia

A complete understanding of the solidification process (nucleation, crystal growth, ripening, vitrification) is one of the long-standing problems in condensed matter physics. The use of colloidal model systems provides an ideal controlled experimental system to reduce this lack of knowledge because the particle movement is much slower than in atomic systems and the crystallisation process can be monitored using optical investigations. Here we present systematic measurements of the solidification kinetics and of the phase behaviour as a function of the particle concentration in nominally one component colloidal model systems of spherical particles. Interestingly we observe a two step behaviour in the nucleation kinetics which was also recently observed in crystallization of proteins and simple atomic liquids.: (i) an induction stage where large numbers of precursor structures are observed; (ii) a conversion stage as precursors are converted to close packed structures. This behaviour is in contrast to the alternative of ordering and densifying at once as assumed in the classical picture of crystallization.

PRL 96, 175701 (2006)

MM 10.5 Mon 17:30 H 1058

From solid solutions to the onset of compound formation and eutectic mixtures in binary charged colloidal suspensions — •Thomas Palberg[1], Nina Lorenz[1], and Patrick Wette[2] — [1]Institut f. Physik, Johannes Gutenberg Universität Mainz, — [2]Institut f. Materialwissenschaft im Weltraum, DLR, Köln

Aqueous colloidal charged sphere suspensions closely mimic the behaviour of metals on a mesoscopic model level. We here ask, whether this also holds for their binary mixtures. We studied the structure, elasticity and solidification kinetics of such mixtures as a function of mol fraction x and total particle density n. At an interaction ratio s = AA/BB = 1 we observe solid solutions of bcc structure, with elasticity and solidification kinetics varying linearly with composition [1]. The onset of compound formation, with extended stability of the crystal phase and corresponding anomalies in elasticity and solidification kinetics occurs at s<0.7. Most recently we found an eutectic behaviour for s=0.55 at x=0.7 with a strongly increased melt stability [2]. Close to the eutectic composition solidification kinetics are dramatically slowed. Our observations are discussed in relation to colloidal mixtures of different interactions (hard spheres, oppositely charged spheres) but moreover carefully analyzed in view of the possible extension of the role of colloids as model systems going from single component to binary systems.

[1] P. Wette, H. J. Schöpe, T. Palberg, J. Chem. Phys. 122, 144901 1-8, (2005).

[2] N.Lorenz, J.Liu, T. Palberg, Colloids Surf. A (at press 2007)

MM 10.6 Mon 17:45 H 1058

Structural changes of undercooled melts in charged colloidal model systems — •Patrick Wette[1], Ina Klassen[1], Dieter M. Herlach[1], Dirk Holland- Moritz[1], Thomas Palberg[2], and Stefan Volkher Roth[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Physik, Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [3]DESY, HASYLAB, 22603 Hamburg, Germany

Colloidal model systems are often used to describe equilibrium properties of fluid and solid materials. Here we used them to study the short range order and the nucleation process in undercooled melts. We employed charged colloidal silica spheres in aqueous dispersion, which enables the precise adjustment of surface charge density and particle interaction via the controlled addition of sodium hydroxide leading to a rich phase behaviour. This colloidal system is characterized by convenient time scales between seconds and minutes and particle distances up to 500nm and is thus accessible by simple, yet powerful optical techniques. By contrast to metals heterogeneous nucleation can either be efficiently suppressed or, if present, clearly discriminated and separated from data evaluation. Microscopy and light scattering yield complementary information on equilibrium properties and crystallization kinetics from real and reciprocal space. Comprehensive measurements of structural changes of the melt with increased undercooling and the corresponding changes of the solidification were carried out by means of the USAXS- technique at HASYLAB (Hamburg).

MM 11: Nanostructured Materials III

Time: Monday 14:45–16:15 Location: H 0107

MM 11.1 Mon 14:45 H 0107

Deformation of Metals at Small Length Scales — •Cynthia Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen

"Smaller is stronger", at least for most metals. When either the sample size or grain size of a metal is decreased below one micrometer, the underlying mechanisms for deformation are changed and almost all mechanical properties - strength in particular - are influenced. Without these effects, many technologies such as microelectronic devices or hard disks would not work. In this presentation, an overview will be given of the observations, proposed mechanisms, and open questions for size effects in metal deformation. In particular, new results from uni-axial compression tests on focused ion beam machined, sub-micron columns confirm the "smaller is stronger" trend, but also challenge the existing models. The models will be critically compared and an outlook of what can be achieved by tailoring length scales in various materials will be presented.

MM 11.2 Mon 15:00 H 0107

Texture and mechanical anisotropy of ultrafine-grained Al alloys produced by accumulative roll bonding — •Juliane Hüttenrauch[1], Werner Skrotzki[1], Carl-Georg Oertel[1], Heinz-Günter Brokmeier[2], Heinz Werner Höppel[3], and Irena Topic[3] — [1]Institut für Strukturphysik, Technische Universität Dresden — [2]GKSS Forschungszentrum, Geesthacht — [3]Lehrstuhl Allgemeine Werkstoffwissenschaften, Universität Erlangen- Nürnberg

The texture of ultrafine-grained Al alloys produced by accumulative roll bonding (ARB) has been measured by neutron diffraction. The starting texture consists of a strong cube component. During ARB this texture breaks down and a texture typical for rolling of face-centred cubic metals with high stacking fault energy develops. The texture after 8 ARB cycles is characterized by the beta-fibre with the Cu component dominating. Moreover, the rotated cube component forms. This component is typical for simple shear which during rolling takes place in the surface layer of the sheets. Based on the Lankford parameter measured the mechanical anisotropy of the advanced metal sheets will be discussed.

MM 11.3 Mon 15:15 H 0107

Strain rate sensitivity of ultrafine-grained Al and Al-Mg-alloys — •Andreas Böhner[1], Johannes May[1], Aferdita Vevecka-Priftaj[2], Heinz Werner Höppel[1], and Mathias Göken[1] — [1]Institute I: General Materials Properties, Department of Materials Science and Engineering, University of Erlangen-Nürnberg, Germany — [2]Department of Physics, Polytechnic University of Tirana, Albania

Nanocrystalline or ultrafine-grained (UFG) metals are known to exhibit very high strength paired with high ductility. In this context, strain rate sensitivity (SRS) is regarded to be the main issue to explain this behaviour. Bulk UFG metals can be achieved by Equal Channel Angular Pressing (ECAP), where the material is deformed by repeated shear deformation. In this contribution, detailed investigations of the SRS of technically pure Al, AlMg and a technologically relevant Al-Mg-alloy (AA6061) were performed. For the precipitation hardenable AA6061-alloy a solution treated and a peak aged state were investigated. The SRS was determined by strain rate jump compression tests which were performed in a temperature range from room temperature (RT) up to 250 °C. It could be shown that an UFG microstructure significantly enhances the SRS, especially at elevated temperatures. The influences of precipitations, microstructure and number of ECAP passes on the SRS and the mechanical properties are also discussed.

MM 11.4 Mon 15:30 H 0107

Influence of high pressure torsion on precipitation in Al-Cu-Mg alloys studied by positron annihilation spectroscopy. — •Wolfgang Lechner[1], Werner Puff[1], Michael Zehetbauer[2], Erhard Schafler[2], and Roland Würschum[1] — [1]Institut für Materialphysik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria — [2]Fakultät für Physik, Forschungsgruppe Physik Nanostrukturierter Materialien, Universität Wien, Boltzmanngasse 5, Universität Wien, 1090 Wien, Austria

High pressure torsion (HPT) may open up an efficient way to refine precipations of supersaturated solutions. In the present work, the influence of HPT on the precipitation in Al-Cu-Mg alloys and on the evolution of the precipitates with subsequent annealing is studied by positron annihilation spectroscopy. HPT is observed to give rise to a fragmentation of metastable nanoscaled precipitates which have formed upon pre-annealing at 200°C (3 hours). Positron lifetime spectroscopy in combination with coincident Doppler broadening of the positron-electron annihilation enables a specific and chemical sensitive distinction between interfacial vacancy-type defects associated with precipitates and the vacancy-type lattice defects formed upon high pressure torsion. Different aging behaviour is observed for undeformed and HPT-deformed samples. Financial support from the Austrian Science Found (FWF) under contracts P18111-N02 and P17095-N02 is gratefully acknowledged.

MM 11.5 Mon 15:45 H 0107

Grain boundary radiotracer diffusion of Ni in ultra-fine grained Cu–1wt.% Pb alloy produced by ECAP — •Jens Ribbe[1], Guido Schmitz[1], Juri Estrin[2], and Sergiy Divinski[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — [2]Department of Materials

Engineering, Monash University, Clayton, Australia

Severe plastic deformation is a promising technique for producing materials with a high hardness and sufficient ductility. Kinetic properties of internal interfaces in such materials with an ultra fine grained microstructure represent one of central issues. The radiotracer technique is applied for measuring Ni grain boundary diffusion in ultra fine grained pure copper materials with different nominal purities and in the Cu–1wt.%Pb alloy produced by equal channel angular pressing (ECAP). The stability of the structure of the nanostructured material was studied by focused ion beam.

The interface diffusion was investigated in the temperature interval from 300 to 520K under the Harrison C type kinetic conditions. Two distinct short-circuit diffusion paths were observed in all materials studied. The first (relatively slower) path corresponds unambiguously to general high-angle grain boundaries with diffusivities which are quite similar to those in their coarse-grained counterparts. The second path is characterized by even higher diffusivities. The measured data favour a one-dimensional but not planar nature of the second diffusion path in the Cu–1wt.%Pb alloy.

MM 11.6 Mon 16:00 H 0107

Three-dimensional tomographic EBSD measurements of the crystal topology in heavily deformed ultra fine grained pure Cu and Cu-0.17wt%Zr obtained from ECAP and HPT — •Anahita Khorashadizadeh, Myrjam Winning, and Dierk Raabe — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Obtaining knowledge on the grain boundary topology in three dimensions is of great importance as it controls the recrystallization and grain growth behaviour of polycrystalline materials. In this study, the three dimensional distribution of grain boundaries and the grain topology of the as-deformed condition have been investigated using three-dimensional orientation microscopy (3D electron backscattering diffraction, EBSD) measurements in ultra fine grained pure Cu and Cu-0.17wt%Zr. Two different methods of severe plastic deformation were used to produce the ultra fine grained structures: equal-channel angular pressing (ECAP) and high pressure torsion (HPT). The experiments are conducted using a dual-beam system for 3D-EBSD. The approach is realized by a combination of a focused ion beam (FIB) unit for serial sectioning with high-resolution field emission scanning electron microscopy equipped with EBSD. The work demonstrates that the new 3D EBSD-FIB technique provides a new level of microstructure information that cannot be achieved by conventional 2D-EBSD analysis. Such information is of great importance in studying metallurgical behaviours which depend on the 3D grain boundary topology (such as grain growth, recrystallization).

MM 12: Nanostructured Materials IV

Time: Monday 16:45–18:15 Location: H 0107

MM 12.1 Mon 16:45 H 0107

Thermal stability and sinterability of segregation-stabilized nanocrystalline alloys — •Lionel Kroner and Carl E. Krill III — Institut für Mikro- und Nanomaterialien, Universität Ulm, D-89081 Ulm

Although it has recently become possible to calculate the mechanical properties of nanocrystalline materials by means of computer simulation, testing these predictions experimentally has been hampered up to now by the difficulty of preparing nanocrystalline samples in bulk form. Ordinary synthesis routes result in powders or thin films, which might then be compacted to a fully dense state via the application of high pressure and temperature; however, the latter generally induces rapid grain growth, resulting in a coarse-grained final product. A potential strategy for sintering to high density without significant grain growth would be to suppress the driving force for coarsening by adding an atomic species that segregates to the grain boundaries. The effectiveness of this approach has already been demonstrated in nanocrystalline Pd alloyed with Zr [1], but the sinterability of such alloy systems remains to be investigated. We have prepared nanocrystalline Ni-Zr alloys by ball milling and examined the thermal stability and densification as a function of Zr concentration. The microstructural evolution that occurred during pressureless sintering was measured by high-temperature x-ray diffraction, and the density following compaction was determined by Archimedes' method.

[1] C. E. Krill III, H. Ehrhardt and R. Birringer, *Z. Metallkd.* **96** (2005) 1134-1141

MM 12.2 Mon 17:00 H 0107

Influence of grain boundaries on the elastic moduli of nanocrystalline palladium — •Manuel Grewer[1], Jürgen Markmann[1], Rainer Birringer[1], and Walter Arnold[2] — [1]Universität des Saarlandes, FR 7.3 Technische Physik, Campus D2.2, 66123 Saarbrücken — [2]Fraunhofer-Institut für zerstörungsfreie Prüfverfahren, Campus E3.1, 66123 Saarbrücken

Grain boundary stress of nanocrystalline Pd has been determined to be on the order of 1 J/m. There is however only scarce knowledge about the interface elastic moduli of nc materials. We take advantage of the recently discovered room temperature (RT) grain growth of nc-Pd and report about in-situ measurements of the transverse and longitudinal velocities of sound and grain size during RT-growth. We deduce the scaling behavior of the overall elastic moduli and discuss a method that enables to extract interface elastic moduli.

MM 12.3 Mon 17:15 H 0107

Investigation of Natural Aging on Precipitation in Al-Mg-Si Alloys — •Cynthia S. T. Chang, Ingmar Wieler, Nelia Wanderka, and John Banhart — Hahn-Meitner-Institut Berlin, Berlin, Germany

The purpose of this work is to investigate the effect of room temperature storage on microstructural evolution in Al-Mg-Si alloys. Alloy H, with 0.4wt%Mg and 0.4%Si and Alloy F, with 0.6%Mg and 0.8%Si were cast in the laboratory. The alloys were then rolled and solution heat treated (SHT) at 540oC. After SHT, the samples were water quenched and then separated into two batches. One batch was artificially aged at 180oC immediately after SHT, while the other batch was subjected to natural aging before it was aged artificially. Microhardness was measured, and Transmission Electron Microscopy (TEM) and Tomographic Atom Probe (TAP) were used to investigate the microstructures of precipitates at different states. From the hardness measurements, it was found that Alloy F possesses a negative strength response which means that its strength is lower when the sample is naturally aged before artificial aging at 180oC. On the other hand, Alloy H possesses a positive strength response. From the TEM and TAP results, the size, shape and density of precipitates were analysed. The results suggest that the negative and positive responses are related to the density and size of the precipitates after natural aging. This influences the nucleation and growth of precipitates during further aging at 180oC.

MM 12.4 Mon 17:30 H 0107

Charakterisierung der Struktur und Dynamik von Ag-Nanoteilchen in Gläsern mittels EXAFS-Spektroskopie — •Holger Kruth, Jörg Haug, Angelika Chassé und Manfred Dubiel — Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II, Institut für Physik

Besondere lineare und nichtlineare optische Eigenschaften können durch den Einbau von Metallnanopartikeln in Gläser erzielt werden. Diese Eigenschaften hängen wesentlich von der Partikelgröße (quantum size effect), der Struktur sowie von Metallpartikel-Glas-Grenzflächeneffekten ab. Deshalb wurde die Röntgenabsorptionsspektroskopie (EXAFS) an der Ag-K-Kante eingesetzt, um die Gitterabstände, die statischen und dynamischen Anteile zum Debye-Waller-Faktor sowie die Kumulanten 3. und 4. Ordnung für Ag-Partikelgrößen bis zu 1 nm zu ermitteln. Mit Hilfe dieser Parameter war eine Beurteilung der Unordnung in der Partikel-Glas-Grenzfläche in Abhängigkeit z.B. vom Herstellungsverfahren möglich. Hierbei wurden in die Berechnung des thermischen Ausdehnungskoeffizienten und der Kumulanten anharmonische und quantenmechanische Effekte im Rahmen einer quantenstatistischen Störungstheorie dritter Ordnung einbezogen [1]. Nur so konnten wesentliche Abweichungen im Vergleich zum kompakten Silber für Partikelgrößen unterhalb von 4 nm nachgewiesen werden.

[1] M. Dubiel, A. Chassé, J. Haug, R. Schneider, H. Kruth in Conference Proc. 882, Melville, New York, 407-409, 2007.

MM 12.5 Mon 17:45 H 0107

Initial stages of mechanical alloying of Fe-Cu-powders investigated by Atom Probe Tomography (APT) — •Catharina Wille[1], Malte Schmidt[1], Taláat Al-Kassab[1], Pyuck-Pa Choi[2], and Reiner Kirchheim[1] — [1]Georg-August-Universität Göttingen, Institut für Materialphysik, Göttingen, Germany — [2]Korea Institute of Science and Technology, Nano-Materials Research Center, Seoul, Korea

Mechanically alloyed powders have been commonly used in industrial application (e.g. spray coatings) for several decades due to their outstanding macroscopic properties. Nevertheless the alloying mechanisms in immiscible systems, characterized by a positive heat of mixing, have not been fully understood so far. To elucidate these associated mechanisms a combination of Atom Probe Tomography (APT), Transmission-Electron-Microscopy (TEM) and X-Ray-Diffractometry (XRD) has been employed to the Fe-Cu-system, which serves as a binary model system.

Powders with low concentrations of the respective minority component ranging from 2.5 at.% to 10 at.% have been investigated, both for Fe-rich and Cu-rich materials. Among the studied milling times of 30min to 50h, this talk will put special emphasis on the shorter times, enabling to gain further insight into the early stages of alloying. Additionally, the effects of impurities such as Oxygen and Carbon on the alloying process will be presented and discussed.

Financial support from the Deutsche Forschungsgesellschaft under contract KI-230/33-1 is gratefully acknowledged.

MM 12.6 Mon 18:00 H 0107

molecular dynamic simulations of homogeneous nucleation of zinc from the supersaturated vapour phase. — •Frank Römer and Thomas Kraska — Institute for Physical Chemistry, University Cologne, Germany

We investigate the homogeneous nucleation of supersaturated zinc vapour by non-equilibrium molecular dynamics simulation [1]. Argon is added to the vapour phase, which acts as inert gas thermostat to remove the latent heat from the forming clusters. Our simulations cover a temperature range from 400 K to 800 K and a supersaturation ranging from log(S) = 2 to 11. We compare two methods for the detection of clusters namely the Stillinger criterion based on atom distances only and the ten Wolde-Frenkel cluster definition requiring at least five next neighbours for each atom to be part of a cluster. To obtain the nucleation rates and the critical cluster sizes, we use the so-called threshold method by Yasuoka and Matsumoto [2] and a mean first passage time method by Wedekind et al. [3]. The simulation results show large deviation to the classical nucleation theory. A similar deviation has been found for experimental data in comparison with the classical nucleation theory. In conclusion the experimental data and simulations are in different domains with respect to supersaturation but both deviate consistently from the classical nucleation theory.

[1] F. Römer, T. Kraska, J. Chem. Phys. in press;
[2] K. Yasuoka, M. Matsumoto, J. Chem. Phys. 109, 8451 (1998);
[3] J. Wedekind et al., J. Chem. Phys. 126, 134103 (2007)

MM 13: Growth

Time: Monday 14:45–16:15 Location: H 0111

MM 13.1 Mon 14:45 H 0111

Triple junction controlled room temperature grain growth revealed by X-ray measurements of nanocrystalline palladium — •Markus Ames, Jürgen Markmann, and Rainer Birringer — Universität des Saarlandes

X-ray measurements at room temperature of nanocrystalline, pure palladium prepared by inert-gas condensation reveal a very fast grain growth from 10 nm up to the instrumental limit of about 60 nm within several hours. Two grain growth regimes have been observed, showing quite different growth kinetics, an intermediate regime in the first 12 h after synthesis which is dominated by an overall decrease of microstrain and only minor grain growth followed by a regime of about 8 h duration that shows linear grain growth kinetics. The latter can neither be explained by a boundary-curvature-driven growth mechanism nor by a vacancy drag model, but in our case by a triple junction controlled grain growth.

MM 13.2 Mon 15:00 H 0111

Monte Carlo simulation and mean-field theory of nanocrystalline grain growth — •Dana Zöllner and Peter Streitenberger — Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

Nanocrystalline grain growth in polycrystals is modelled under the assumption that the mobility of grain boundaries is limited at small grain sizes. In particular, following the works of Gottstein, Shvindlerman, Novikov and others, it is assumed that the grain boundary mobility depends, for two-dimensional grain growth, on the triple junction distance.

Based on this assumption a modified Monte Carlo Potts model algorithm is presented allowing the simulation of grain growth controlled by size effects. For initially very small grains linear grain growth kinetics is observed, which is associated with an approximately quasi-stationary self-similar grain size distribution shifted to smaller relative grain sizes. This linear growth regime can adequately be described by a statistical mean-field theory yielding an analytical grain size distribution function that is in good agreement with the simulation results.

MM 13.3 Mon 15:15 H 0111

Kinetics of grain growth in nanocrystalline Fe at low annealing temperatures — •Heiko Paul and Carl E. Krill III — Institut für Mikro- und Nanomaterialien, Universität Ulm, Albert-Einstein-Allee 47, D-89081 Ulm

The migration rates of curved grain boundaries (GB) and triple junctions (TJ) manifest different dependencies on the average grain size $\langle R\rangle$, implying that there may be a critical grain size $\langle R\rangle_c$ below which the overall growth kinetics are controlled by TJ migration. If the activation enthalpy for TJ migration is significantly higher than that for GB migration, then a linear growth law is expected when $\langle R\rangle < \langle R\rangle_c$, whereas the well-known parabolic growth behavior should still obtain when $\langle R\rangle > \langle R\rangle_c$. To test this hypothesis, we carried out long-term *in situ* annealing experiments on highly pure samples of nanocrystalline Fe. Grain growth was measured in a laboratory x-ray diffractometer (XRD) equipped with a heating stage and a position-sensitive detector. By fitting linear and parabolic growth models to isothermal grain-growth curves recorded at temperatures between 409°C and 482°C, we were able to extract activation enthalpies for initial and late-stage coarsening, observing a decrease suggestive of a transition between TJ-controlled and GB-controlled growth. Additional microstructural analysis was performed to verify the average grain-size values calculated from the XRD measurements.

MM 13.4 Mon 15:30 H 0111

On the role of elastic strains in the precipitation of second phases — •Volker Mohles, Emmanuel Jannot, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen

The use of Green functions allows the efficient resolution of elasticity problems. However, previous attempts to use this methodology to derive the stored elastic energy in a solid solution haven't been fully successful. For example, the one atom thick plate morphology of GP zones in Al-Cu alloys can't be reproduced using the theory developed by Khachaturyan. The present work provides an explanation for this discrepancy. An improved version of the Microscopic Elasticity theory will be presented. Calculations indicate that this improvement reduces the error generated by the use of Green functions to less than 2% compared to Molecular Statics relaxations. Consequently, the role of elastic strains for the precipitation of second phases can be evaluated more precisely. Simulations for model materials revealed that elastic strains should be first considered as a positive driving force for nucleation. For example, the energy gain offered by the concentration of point defects like solute atoms explains the stability of second

phases up to the melting point of aluminum for solute atoms having a 10% lattice mismatch. Using the improved theory, new insight on the factors explaining the precipitate morphology is provided. This work confirms the importance to consider elastic anisotropy.

MM 13.5 Mon 15:45 H 0111

Optical-image-furnace growth and characterisation of transition metal Heusler compounds — •Andreas Neubauer, Christian Franz, and Christian Pfleiderer — Physik-Department E21, Technische Universität München, D-85747 Garching, Germany

Both full (X_2YZ) and half (XYZ) Heusler compounds offer a huge variety of electronic and magnetic phenomena [1], e.g., half-metallic ferromagnetism, the magnetic shape memory effect, heavy-fermion behavior and unusual antiferromagnetic states. To gain further information about the physical properties of Heusler compounds detailed studies on high quality single crystals are essential. In recent years it has been found that optical as opposed to RF heated floating zone crystal growth produces very high quality single crystals [2]. Minimizing sample contamination (e.g. oxygen) is thereby a key prerequisite for high quality crystals. Going beyond present day technology [2], we set up a commercial image furnace for use with ultra-high vacuum and ultra-pure inert gas atmosphere by converting it to all metal-sealing. The furnace may be baked out to reduce any residual contamination by the system. To prepare polycrystalline feed rods for single-crystal growth we also set up a RF heated high-purity casting assembly employing a Hukin-type cold-crucible. Single crystals of the Heusler compounds Mn_3Si and Fe_2TiSn were grown and characterised. We present a structural analysis as well as transport and thermodynamic bulk properties. [1] for a review see e.g., I. Galanakis et al, cond-mat/0709.4183v2 (2007). [2] G. Behr, W. Löser, Recent Res. Devel. Crystal Growth **4**, 129 (2005).

MM 13.6 Mon 16:00 H 0111

Influence of Strain on Kinetics of Nonisothermal Solid-Solid Phase transitions — •Michael Fleck, Efim Brener, Robert Spatschek, and Guillaume Boussinot — Institut für Festkörperforschung, Forschungszentrum 52425 Jülich

Structural phase transitions in solids involve a discontinuous change in the lattice structure, leading to the presence of elastic deformations. In some cases, these effects are of minor influence and can be ignored, but nevertheless for many applications the elastic strain causes qualitatively new and observable effects.

A motion of the interface due to first order phase transitions is a source of latent heat due to the finite entropy difference of the two phases. This heat has to be transported away from the interface before further phase transformations can take place. From solidification or melting processes it is known, that these kinds of thermal effects can cause interface instabilities leading to dendritic growth, which is very important for many metallurgical applications.

We derive a thermodynamically consistent phase field model for nonisothermal solid-solid phase transitions, to be able to investigate the coupled influence of elastic and thermal effects on the kinetics of solid-solid phase transitions. We show results from simulations with different geometries and boundary conditions. In particular, we investigate the steady state growth in a narrow channel, and compare the results to analytical predictions for the region far behind the tip.

MM 14: Electronic Properties I

Time: Monday 16:45–18:30 Location: H 0111

MM 14.1 Mon 16:45 H 0111

Band structure mapping and calculations of metallic $MoTe_2$ — •Thorsten Zandt, Robert Heimburger, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

Calculations of the electronic structure have been performed using an self-consistent full potential linearized augmented-plane-wave (FP-LAPW) method in order to compare $MoTe_2$ in its two metallic forms, i. e. β- and Td-$MoTe_2$. In β- and Td-$MoTe_2$ the metal atom is displaced from the centre of an octahedron of Te atoms, and metal-metal chains with bond lengths only slightly longer than in the elemental metals occur along the layers. Thus one can guess that β- and Td-$MoTe_2$ are normal metals. From the band structure calculations we found that only few bands cross the Fermi energy. In the total DOS this leads to a distinct minimum at the Fermi energy. Therefore our interpretation is that $MoTe_2$ forms semimetals rather than metals, which is in good agreement with observed low conductivity [1]. The electronic structure between the monoclinic α-phase and orthorhombic β-phase of $MoTe_2$ is essentially unchanged. We discuss the theoretical results in comparison with experimental valence band studies using angle-resolved photoelectron spectroscopy taken from measurements at BESSY II.

[1] T. Zandt, H.Dwelk, C. Janowitz, and R. Manzke, Journal of Alloys and Compounds, 442, 216-218 (2007)

MM 14.2 Mon 17:00 H 0111

Spectral-weight analysis from ellipsometric spectroscopy on FeSi single crystals — •Dirk Menzel[1], Paul Popovich[2], Alexander Boris[2], Ana Maria Racu[1], and Joachim Schoenes[1] — [1]TU Braunschweig, Institut für Physik der Kondensierten Materie — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

One of the key arguments of the supporters of the description of FeSi as Kondo insulator stems from reflectivity measurements. After Kramers-Kronig analysis (KKR) of these data the resulting optical conductivity spectra in some cases [1] show a loss of spectral weight when the gap opens at low temperature, which is not recovered in the neighborhood of the gap, while in some cases it does not [2]. Since the determination of absolute conductivity values from reflectivity spectra is problematic, we have undertaken ellipsometry measurements from the far-infrared to the UV spectral range, giving directly - without KKR - the optical conductivity. We find that the spectral weight is not compensated up to 2.5 eV. At low temperatures the indirect gap amounts to 33 meV and is filled at a temperature of about 250 K. This is in agreement with our recent Raman investigations indicating a change in the effective masses of the charge carriers as function of temperature which results in a shift of the chemical potential towards the valence band [3]. It is discussed if an interaction among d-electrons can be the origin of the widely spread spectral-weight recovery.

[1] Z. Schlesinger et al., Phys. Rev. Lett. **71**, 1748 (1993).
[2] L. Degiorgi et al., Europhys. Lett. **28**, 341 (1994).
[3] A. M. Racu et al., Phys. Rev. B **76**, 115103 (2007).

MM 14.3 Mon 17:15 H 0111

Parity of substrate bands probed by quantum-well states of overlayer — •Denis Vyalikh[1], Yuriy Kucherenko[2], Frederik Schiller[3], Matthias Holder[1], Andreas Kade[1], Serguei Molodtsov[1], and Clemens Laubschat[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institute of Metal Physics, National Academy of Sciences of Ukraine, UA-03142 Kiev, Ukraine — [3]Departamento de Fisica de Materiales, Universidad del Pais Vasco, E-20018 Spain

Quantum-well (QW) states in metallic nanostructures are objects of continued interest and exhibit permanently novel fascinating phenomena. In the present contribution we demonstrate by means of by angle-resolved photoelectron spectroscopy (ARPES) study of Ag/W(110)supported by Layer Korringa-Kohn-Rostoker (LKKR) calculations that energy overlap of QW and substrate bands of the same parity lead to the formation of broad hybridization gaps around the k-point of the crossings. Since the symmetry properties of two-dimensional QW bands can easily be determined, they can successfully be used as fingerprints to probe parity of substrate bands. The parity data provide information about site-specific localization of electron densities that may be used, e.g. to understand interactions in correlated materials like high-temperature superconductors electron-phonon coupling) or heavy-fermion systems (f-d hybridization). References: 1) D. V. Vyalikh et al., Phys. Rev. B 76, 153406 (2007).

MM 14.4 Mon 17:30 H 0111

High Kinetic Energy Photoelectron Spectroscopy at BESSY — •Mihaela Gorgoi[1], Svante Svensson[2], Marcel Mertin[1], Franz Schäfers[1], and Walter Braun[1] — [1]BESSY GmbH, Berlin, Germany — [2]Uppsala University, Uppsala, Sweden

The present work will show the investigation possibilities offered by

the recently developed high kinetic energy photoelectron spectroscopy (HIKE) at the Berliner synchrotron light source. Hard x-ray photoemission has proven to be a non-destructive depth profiling tool for the characterisation of bulk electronic properties of different types of materials as well as interface properties of organic and inorganic thin films and multilayers. The HIKE end station operates at the KMC-1 bending magnet beamline. Electron spectra have been recorded using x-ray energies from 2 keV up to 12 keV excitation energies. Exemplifying results will be given in order to demonstrate the performance of the technique and its advantages.

MM 14.5 Mon 17:45 H 0111

Global exploration of the energy landscape of solids on the ab initio level — •Klaus Doll, J Christian Schön, and Martin Jansen — Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany

Predicting which crystalline modifications can be present in a chemical system requires the global exploration of its energy landscape. Due to the large computational effort involved, in the past this search for sufficiently stable minima has been performed employing a variety of empirical potentials and cost functions followed by a local optimization on the ab initio level. However, this entails the risk of overlooking important modifications that are not modeled accurately using empirical potentials. In order to overcome this critical limitation, we develop an approach to employ ab initio energy functions during the global optimization phase of the structure prediction. As an example, we perform a global exploration of the landscapes of LiF [1] and BN on the ab initio level and show that the relevant crystalline modifications are found during the search.

[1] K. Doll, J. C. Schön and M. Jansen, Phys. Chem. Chem. Phys., in press

MM 14.6 Mon 18:00 H 0111

Calculations of the force-constant tensor within the KKR Green's function method — •Sergiy Mankovsky and Hubert Ebert — Dept. Chemie und Biochemie/Phys. Chemie, LMU München, Butenandtstr. 11, D-81377 München, Deutschland

We present a formalism for the calculation of the force-constant tensor within the KKR Green's function method. As a primary information the formalism gives the real-space force-constant tensor, i.e. the pairwise interaction parameters, on the basis of ab-initio electronic structure calculations. Accordingly, the technique is applicable in principle to any system as for example solids, surfaces and nanostructures. In addition this feature opens the way for a number of interesting applications. First results for the force-constant tensor of solid state systems will be presented together with corresponding results for the phonon dispersion relation. Comparison will be made with experiment and results of other theoretical works.

MM 14.7 Mon 18:15 H 0111

Residual resistance calculations of transition metal alloys including short-range ordering effects — •Stephan Lowitzer[1], Diemo Ködderitzsch[1], Hubert Ebert[1], Julie Staunton[2], and Paul Tulip[2] — [1]Department Chemie und Biochemie, LMU München, Butenandstr. 11, 81377 München — [2]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

The residual resistance (at T = 0K) of Cu_xZn_{1-x} and Ag_xPd_{1-x} has been calculated. For these calculations the Kubo-Greenwood formalism has been employed. The electronic structure calculations are based on the fully relativistic Korringa-Kohn-Rostoker (KKR) band structure method in connection with the coherent potential approximation (CPA) alloy theory. To deal with short-range ordering effects we used the more elaborated nonlocal coherent potential approximation (NL-CPA). Our results show the expected behavior of decreasing resistivity when one includes short-range ordering effects in good agreement with experimental data.

MM 15: HV Meyer

Time: Tuesday 9:30–10:00 Location: H 1058

Invited Talk MM 15.1 Tue 9:30 H 1058

Phase Transformations in Thin Films and Near-Surface Regions: Stimulation and Application — •Dirk Carl Meyer — Technische Universität Dresden, Institut für Strukturphysik

In thin films and near-surface regions of materials the variety of structural phases - due to the influence of surface energy or strain - can be extended significantly. Beyond, a lot of preparation methods is characterised by a processing far from thermodynamic equilibrium, allowing for stabilisation of crystalline metastable states. Additionally, regions near electrodes or in direct contact with atmosphere can exhibit a structural behaviour quite different from that of states which are characteristic for thermodynamic equilibrium of volume materials. Generally speaking, for this kind of materials only the tendency of reactions can be obtained from studies of thermodynamic equilibrium phase diagrams. The influence of external fields and any kind of energy support in turn can yield to other metastable states which represent an energetically more suitable situation. In certain cases this ripening can be reversed. The investigation of this variety of structures and transitions is of high interest due to the well-known fact that a new phase originates new properties what is outlined with respect to technical applications.

MM 16: SYM Phase Transformations in Metallic Melts V

Time: Tuesday 10:15–11:15 Location: H 1058

MM 16.1 Tue 10:15 H 1058

Einfluss der Schmelzkonvektion auf das Gefüge von NdFeB- und TiAl-Legierungen — •Regina Hermann[1], Gunther Gerbeth[2], Kaushik Biswas[1], Octavian Filip[3] und Victor Shatrov[2] — [1]IFW Dresden — [2]FZ DD-Rossendorf — [3]Uni Erlangen

Die magnetischen und mechanischen Eigenschaften technisch relevanter Nd-Fe-B und Ti-Al Legierungen hängen stark von Gefüge und Volumenanteil der properitektischen Phase ab. Auf der Basis numerischer Simulationen der Schmelzkonvektionsmoden in einer induktiv beheizten Schmelze, wurden neuartige Versuchsaufbauten entwickelt, die die Modifizierung der Konvektion in einer Metallschmelze ermöglichen. Dies sind ein Aufbau zur erzwungenen Schmelzrotation in einem Tiegel und eine modifizierte Floating-Zone-Anlage. Die erzwungene Schmelztiegelrotation führt in Übereinstimmung mit der Simulation zu einer starken Reduzierung der Konvektion und des Volumenanteils der properitektischen Phase mit zunehmender Frequenz, einhergehend mit einer Verringerung der Abstände der sekundären Dendritenarme. Eine Floating-Zone-Anlage mit einem patentierten Doppelspulensystem stellt eine zusätzliche wohl definierte elektromagnetische Kraft zur Verfügung, über die in einem weiten Bereich sehr intensive bzw. stark verringerte Strömung eingestellt werden kann. Die mechanischen Eigenschaften unter starker Schmelzkonvektion erstarrter TiAl-Legierung zeigten eine signifikant höhere plastische Verformbarkeit. Bei beiden Legierungen wurde mit zunehmender Rührwirkung ein Wechsel der Morphologie von dendritisch zu globular beobachtet.

MM 16.2 Tue 10:30 H 1058

Untersuchung der Phasenbildung in Nd-Fe-B-Schmelzen mit Synchrotron-Strahlung — •Thomas Volkmann[1], Jörn Strohmenger[1,2], Oliver Heinen[1], Dirk Holland-Moritz[1] und Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln — [2]Institut für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum

Die Phasenbildung in unterkühlten Nd-Fe-B-Schmelzen wurde an der European Synchrotron Radiation Facility (ESRF) durch energiedispersive Beugung an elektromagnetisch levitierten Proben unter-

sucht. Es zeigt sich, dass die Erstarrung der unterkühlten Schmelze durch γ-Fe eingeleitet wird, auch bei Temperaturen, bei denen nur die $Nd_2Fe_{14}B_1$-Phase stabil ist. Es gelang, die Kristallisation einer metastabilen Phase bei tiefen Unterkühlungen direkt zu beobachten.

Dieses Vorhaben wurde von der Deutschen Forschungsgemeinschaft unter dem Kennzeichen HE 1601/14 und dem ESRF unterstützt.

MM 16.3 Tue 10:45 H 1058

Nanosized magnetisation density profiles in hard-magnetic NdFeCoAl glasses — •A. Wiedenmann[1], O. Perroud[1], M. Stoica[2], and J. Eckert[2] — [1]HMI-Berlin, Glienickerstr. 100, 14109 Berlin — [2]IFW-Dresden, P.O. Box 270116, 01171 Dresden

Nd-Fe-Co-Al alloys have a high glass forming ability and show hard magnetic behavior at room temperature. The aim of the present SANS investigation was to establish structural and magnetic units in the alloys on a nanometer length scale and correlate them with the observed magnetic properties. $Nd_{80}Fe_{20}$ and $Nd_{60}Fe_xCo_{30-x}Al_{10}$ cylinders with x=0, 7.5 and 20 have been produced by mold casting with different diameters and have been investigated by SANS, SEM/TEM and magnetization measurements. The microstructure consists of a Nd-rich matrix, a Fe-rich partially amorphous phase and of nanosized Nd particles. The magnetisation show two transition temperatures: T_{c1} ∼40K corresponds to the ordering of the magnetic moment in the Nd phases and and T_{c2} ∼500K to the Curie temperature of the Fe-rich phase. The low magnetic scattering contribution has been extracted beside the strong nuclear scattering by using polarized neutrons. It turned out that the Fe-rich phase is essential for the hard magnetic properties of the alloys where the nanoparticles play an important role, while the Fe free alloy is soft magnetic. The magnetization density profil depends on T: Well below T_{c1} the local magnetization of the nanosized particles is higher than that of the ferromagnetic matrix while above T_{c1} they are paramagnetic and act more efficiently as pinning centers for the magnetic domains, which enhance the coercivity above T_{c1}.

MM 16.4 Tue 11:00 H 1058

Microstructure and properties of binary $Nd_{80}Fe_{20}$ alloys with Ga additions — •Mihai Stoica[1], Mahesh Emmi[1,2], Shanker Ram[2], Albrecht Wiedenmann[3], Olivier Perroud[3], and Jürgen Eckert[1] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270016, D-01171 Dresden, Germany — [2]Materials Science Centre, Indian Institute of Technology, Kharagpur 721302, India — [3]Hahn-Meitner Institute Berlin, Glienickerstr. 100, D-14109 Berlin, Germany

The microstructures upon solidification are diverse and depend primarily on the alloy composition and the applied cooling rate. Fast cooled binary $Nd_{80}Fe_{20}$ shows hard magnetic properties which can be tuned by properly adjusting the cooling rate. Additions of elements like Ga induce a variation in structure and as a result the magnetic properties change. The investigated alloys contain 4, 8 and 12 at.% Ga. From every composition different samples were produced. Melt spinning was used to produce 4 mm wide and 30 μm thick ribbons and rods with diameters of 3, 5 and 7 mm were cast by copper mould casting. The structure of the samples was investigated by X-ray diffraction and electronic microscopy and the thermal stability was checked by differential scanning calorimetry (DSC). We will discuss the microstructure formation for different samples as a function of two parameters: the composition and the cooling rate. Additionally, the magnetic behaviour of the quenched samples will be presented and discussed in the light of changes in microstructure. The work was supported by the German Science Foundation (DFG) via the DFG priority program Phasenumwandlungen in mehrkomponentigen Schmelzen.

MM 17: SYM Phase Transformations in Metallic Melts VI

Time: Tuesday 11:30–13:00 Location: H 1058

MM 17.1 Tue 11:30 H 1058

Modeling elasticity effects in pattern formation during alloy solidification — Bo Liu[1], •Klaus Kassner[2], Robert Spatschek[3,4], and Clemens Müller-Gugenberger[4] — [1]AG Mathematische Modellierung, MPI für Marine Mikrobiologie, Bremen — [2]Institut für Theoretische Physik, Otto-von-Guericke Universität, Magdeburg — [3]Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, Massachusetts, USA — [4]Institut für Festkörperforschung, Forschungszentrum Jülich

We have developed a series of phase-field models allowing to simulate various aspects of strain-induced effects on alloy solidification. On the one hand, we include compositionally induced stresses in a phase-field model describing growth of dilute alloys. Special care is taken to obtain a viable thin-interface limit, i.e., we eliminate artificial effects of interface stretching, surface diffusion, and interface dissipation by an appropriate choice of phase-field functions and parameters. Simulations of directional solidification in a parameter range discussed by Spencer et al. [1] in terms of a linear stability analysis reveal oscillatory standing wave modes as the preferred dynamic state. On the other hand, after realizing that past models are flawed, we have created asymptotically correct phase-field models for the simulation of surface diffusion under stress, which may become important in solidification when micro-crack formation plays a role.

[1] B.J. Spencer, P.W. Voorhees, S.H. Davis, G.B. McFadden, *Acta metall. mater.* **40** 1599 (1992).

MM 17.2 Tue 11:45 H 1058

Elastic effects on phase transitions in multicomponent alloys — •Denis Pilipenko, Robert Spatschek, Efim Brener, Heiner Mueller-Krumbhaar, and Clemens Mueller-Gugenberger — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425Jülich, Germany

We report on our activities concerning the influence of elastic effects on multicomponent alloys, which can lead to long-range interactions and the appearance of unexpected dynamical behaviors. We present a continuum theory to describe elastically induced phase transitions between solid and melt phases, which is simulated both by phase field and sharp interface methods. For the particular case of diffusionless phase transitions in solids, where structural and density differences provoke significant strain effects, we predict the macroscopic growth in a strip geometry, which can lead to the emergence of twin boundaries. In the limit that one phase is very soft, we obtain a self-consistent macroscopic model for fast fracture processes, which is based on the Asaro-Tiller-Grinfeld instability. Here we demonstrate that sharp-interface and phase field predictions are in very good agreement despite the large lengthscale gaps that are intrinsic to this problem. Finally, we briefly present recent results concerning the diffusion-limited propagation of a melt phase along an inter-phase boundary and melting in eutectic and peritectic systems.

MM 17.3 Tue 12:00 H 1058

Nonequilibrium crystal growth: a comparison of molecular dynamics and phase-field simulations — •Denis Danilov[1], Britta Nestler[1], Alexander Mirzoev[2], and Ilya Maltsev[2] — [1]Hochschule Karlsruhe, Karlsruhe, Germany — [2]South-Ural State University, Chelyabinsk, Russia

Melting and crystallization are of fundamental interest in condensed matter physics. We employed molecular dynamics (MD) simulations to investigate nonequilibrium behavior of crystallization with a simple system: the Lennard-Jones (LJ) 6-12 potential. Although quantitatively, LJ model at best applies to noble gases, it is used as a generic model for simple close-packed systems. Simulations of crystal growth from the melt were performed in the (100) direction, measuring the growth velocity as a function of the undercooling. Different definitions of the order parameter that discriminates between the solid like and liquid like particles in the simulation box have been considered. The influence of the termostat type on the growth kinetics has been tested, showing the crucial role that the approximation of the release of the latent heat plays in MD modeling of crystal growth. The MD results are compared with phase-field simulations where input model parameters were obtained from atomistic simulations.

MM 17.4 Tue 12:15 H 1058

Modelling of dendrite growth and fragmentation in multicomponent melts — Peter Galenko and •Dieter Herlach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany

A progress reached in direct experimental measurements of non-equilibrium solidification allows for developing and verifying theoretical models in a wide range of undercooling. Both sharp-interface model and diffuse interface model are applied to solidification of pure (one component) melts, binary alloys (both dilute and concentrated), and ternary diluted alloys. The current theories of dendritic growth based on these models correlate the undercooling to the dendrite growth velocity. It is shown that the sharp-interface model reasonably predicts kinetics of dendritic solidification in agreement with the experimental data obtained by the methods of in situ diagnostic (e.g., using high-speed camera). In addition to the predominant effect of diffusion transport of atoms and conductive transport of heat on growth kinetics, convection of the liquid may quantitatively influence on the growth and fragmentation of dendrites. Combined with in situ diagnostic of solidification, advanced computer modelling of microstructure formation on the basis of experimentally proven physical models allows for developing the perspective of virtual materials design of high functional materials. Financial support by DFG under SPP-1120 through the project DFG-HE1601/13 is acknowledged.

MM 17.5 Tue 12:30 H 1058

Dendritic solidification in the diffusive regime and under the influence of buoyancy driven melt convection — •Ingo Steinbach and Markus Apel — RWTH-Aachen, Access e.V.

Simulations of dendritic solidification in binary and ternary alloys in the diffusive regime and under the influence of buoyancy driven melt convection are performed using a quantitative phase-field model. At first, in the diffusive regime rapid solidification into a highly undercooled melt of ternary Ni-Al-Zr is investigated and compared to levitation experiments and sharp interface calculations. Secondly, the stability of dendritic arrays dependent on the primary spacing is investigated for a binary Al-Cu alloy under directional solidification conditions. Thirdly, melt convection driven by solutal buoyancy is introduced to the latter case and the influence of buoyancy on the spacing selection is discussed. A scaling relation for the dependence of primary spacing on the gravity level is derived and compared to experimental results from centrifugal casting under increased gravity.

MM 17.6 Tue 12:45 H 1058

Stationäre und instationäre Morphologieentwicklung bei gerichteter Erstarrung ternär-eutektischer Legierungen — •Bernd Böttger, Victor Witusiewicz, Markus Apel, Ulrike Hecht und Stephan Rex — access, Aachen, Germany

In diesem Beitrag werden Ergebnisse zu Erstarrungsexperimenten, zum thermodynamischen Assessment sowie zur Phasenfeld-Simulation in ternär-eutektischen Legierungssystemen vorgestellt. In einem ersten Schritt wurde die vollständige thermodynamische Beschreibung der Systeme Ag-Cu-Zn und Bi-In-Sn erarbeitet, für die nur bruchstückhafte Informationen vorlagen. Hierfür wurden Experimente durchgeführt. Diese Daten stehen somit als CalPhaD-Datenbanken zur direkten Ankopplung an die Simulation zur Verfügung.

Experimente zur gerichteten Erstarrung wurden sowohl in der klassischen Bridgman-Technik als auch als pseudo-2D-Experimente in dünnen Glaskapillaren durchgeführt. Für letztere Technik wurde eigens ein Mikro-Bridgman-Aufbau entwickelt, der eine in-situ-Beobachtung der Gefügebildung erlaubt. Dadurch wurden insbesondere die Durchführung transienter Experimente und die Beobachtung instationärer Mikrostukturen im Legierungssystem In-Bi-Sn möglich.

Die Anwendung der Phasenfeldmethode zur Gefügesimulation führte zu einem neuen Verständnis der stationären und instationären Erstarrungsprozesse in 2D und 3D. Für In-Bi-Sn konnte ein quantitativer Vergleich mit pseudo-2D-Experimenten durchgeführt werden, der auch die indirekte Bestimmung von Diffusionskoeffizienten und Grenzflächenenergien ermöglichte.

MM 18: SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling I

Time: Tuesday 10:15–11:15 Location: H 0107

Invited Talk MM 18.1 Tue 10:15 H 0107

Local Probing of Magnetic Properties by Electron Microscopy — •Josef Zweck — NWF II - Physik, Universität Regensburg

Presently, huge efforts are made to combine magnetism with sensors or other electronic devices, or to simply use patterned magnetic materials for data storage. Frequently cited applications include GMR-based magnetic field sensors, spin transistors or "spintronics"and magnetic random access memories (MRAMs). The existing as well as future applications require the ability to manufacture magnetic devices far below the micrometer range and to characterize them.

One of the few techniques capable to investigate magnetic properties of **individual** magnetic particles with both high lateral (5 nm) and magnetic (2.5 Tnm) resolution is electron microscopy. The talk will demonstrate the ability to characterize individual magnetic particles and the dependence of the magnetic properties on their size and geometry. While control of size and shape can lead to the design of magnetic properties (single domain switching, taylored hysteresis loops, superparamagnetic behaviour) the lack of precise control can lead to arbitrary switching behaviour and unexpected domain structures.

MM 18.2 Tue 10:45 H 0107

Nanoscale characterization of electroplated, thick permalloy films — •Michael R. Koblischka[1], Saleh Getlawi[1], Martin Theis[2], Anjela Koblischka-Veneva[3], Monika Saumer[2], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, P.O.Box 151150, D-66041 Saarbrücken, Germany — [2]Department of Microsystems Technology, University of Applied Sciences, Campus Zweibrücken, Amerikastrasse 1, D-66482 Zweibrücken, Germany — [3]Institute of Functional Materials, Saarland University, P.O.Box 151150, D-66041 Saarbrücken, Germany

Permalloy (Py) samples were fabricated by means of electroplating, (1) a patterned Py film on a Si wafer and (2) a NiFe foil. The grain sizes of the samples were measured employing AFM and TEM to be of the order of 50 nm (type (1)) and around 200 nm (type (2)). TEM further reveals that along the substrate, larger elongated grains are located, and after this layer, the regular grain growth sets in. Electron backscatter diffraction (EBSD) was employed to obtain Kikuchi patterns of Py which can be unambiguously identified due to the thickness of the samples, and via them the individual crystallographic orientation of the grains. The samples required a mechanical polishing procedure down to 40 nm colloidal silica particles, yielding a smooth surface with a roughness of nm dimensions. With the recently achieved high spatial resolution of the EBSD technique, the individual grain orientations in such samples can be determined for the first time. The EBSD results reveal a fibre-texture of the electroplated Py.

The EBSD work is supported by the DFG (Mu959/19).

MM 18.3 Tue 11:00 H 0107

Misorientations in magnetite thin films studied by electron backscatter diffraction — Anjela Koblischka-Veneva[1], •Michael R. Koblischka[2], Sunil Arora[3], Shane Murphy[3], Frank Mücklich[1], Uwe Hartmann[2], and Igor Shvets[3] — [1]Institute of Functional Materials, Saarland University, P.O.Box 151150, — [2]Institute of Experimental Physics, Saarland University, P.O.Box 151150, — [3]SFI Nanoscience Laboratory, Trinity College, Dublin, Dublin 2, Ireland

Magnetite thin films grown on [0 0 1] oriented MgO substrates are analyzed by means of electron backscatter diffraction (EBSD) analysis. Upon annealing in air, the magnetic properties of the magnetite thin films were found to change considerably. Using EBSD analysis, we find that after 3 minutes annealing, most of the misorientations around 30°-40° are vanished, and some areas with high misorientation angles more than 45° remain. These misoriented grains form small islands with a size of about 100 nm. The size and distribution of these islands correspond well to the observations of antiferromagnetic pinning centers in the magnetic domain structures carried out by magnetic force microscopy (MFM) on the same samples. EBSD can recognize maghemite particles embedded within the magnetite matrix. The detected maghemite particles (4 % of the total) are found to be very small (˜50 * 100 nm in diameter), but also clusters of them are detected. It is important to note that their presence is also causing misorientations within the magnetite matrix. The quality of such multi-phase EBSD analysis is discussed in detail.

MM 19: SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling II

Time: Tuesday 11:30–13:00 Location: H 0107

Invited Talk MM 19.1 Tue 11:30 H 0107

Atom Probe Characterization of Magnetic Thin Film Structures — •David Larson — Imago Scientific Instruments, Madison, WI USA

Improvements in the properties of nanoscale devices based on giant magnetoresistance or tunnel magnetoresistance depend on the capabilities of researchers to design, fabricate, and test such devices. Optimization of these capabilities are intimately tied to the feedback provided by the quality and quantity of available microscopic characterization. This work presents examples of the use of atom probe tomography to investigate microstructure for a variety of nanomagnetic thin film structures including multilayers, spin valves and tunnel barriers. Examples of interface characterization methods including a discussion of buried interface "roughness" will be given. Comparison of interfacial nature of experimental atom probe data and molecular dynamics simulation of thin film growth of a CoFe/Cu layered structures will also be presented.

Invited Talk MM 19.2 Tue 12:00 H 0107

Thermal stability and reaction of GMR sensor materials — •Vitaliy Vovk[1], Constantin Ene[2], and Guido Schmitz[3] — [1]Department of materials, University of Oxford, Parks Road 3PH, U.K. — [2]Institut für Materialphysik, Univ. Goettingen, Friedrich-Hundt-Platz 1, 37077 Göttingen, Germany — [3]Institut für Materialphysik, WWU Muenster, Wilhelm-Klemm-Str. 10, 48149 Muenster, Germany

State-of-the-art GMR sensors usually consist of thin film multilayers with a periodicity of a few nanometers only. The significant contribution of interfaces makes these nano-scaled materials inherently unstable. In the talk, the stability and thermal reaction of Py/Cu (Py stands for Ni81Fe19) and Co/Cu magneto resistive systems is addressed.

Thin film multilayers are analysed by wide angle atom probe tomography (WATAP). The different thermodynamics of the studied systems causes different mechanisms of GMR degradation. In the Py/Cu system, GMR deterioration occurs due to short range mixing at the layer interfaces, caused by gradient energies and quantitatively described by Cahn-Hilliard theory. In contrast, this mechanism is not observed in Co/Cu multilayers up to temperatures of 450°C. Instead, ferromagnetic bridges along grain boundaries through Cu appear at even higher temperatures.

Besides the mixing reaction, a recrystallization transforming the layer texture is observed in both metallic systems. Elasto-mechanic calculations demonstrate that this transformation is due to elastic anisotropy.

Invited Talk MM 19.3 Tue 12:30 H 0107

Solid state reactions at the interface of Heusler alloy films — •Hans-Joachim Elmers[1], Andres Conca[1], Tobias Eichhorn[1], Andrei Gloskovskii[2], Kerstin Hild[1], Gerhard Jakob[1], Martin Jourdan[1], and Michael Kallmayer[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz, Germany — [2]Institut für Anorganische und Analytische Chemie Johannes Gutenberg-Universität, D-55099 Mainz, Germany

Magnetic and structural properties on a nanoscale are of vital interest for data storage and actuator applications of magnetic thin films. Half-metallic Heusler alloy films offer new routes for the development of devices based on spin transfer mechanisms. Ferromagnetic shape memory alloy films provide potential applications exploiting their huge magnetically induced length change. The control of interface properties of these complex alloys is crucial for future applications. We show that x-ray absorption spectroscopy can be used as an efficient tool for the determination of element-specific magnetic and structural properties both in the bulk and at buried interfaces. We present results for the variations of orbital and spin moments at the martensitic phase transition of Ni_2MnGa. As an example for the modification of interface properties, we present results on the solid-state reaction at the interface of Heusler alloys and Al. Micro-spectroscopy using photoemission electron microscopy (PEEM) reveals an inhomogeneous interface reaction with reaction nuclei separated on a micron length scale.

MM 20: Electronic Properties II

Time: Tuesday 10:15–11:30 Location: H 0111

MM 20.1 Tue 10:15 H 0111

Non local exchange and correlations in Fe — •Gernot Stollhoff — MPI f. Festkörperforschung, Heisenbergstr.1, D 70569 Stuttgart

Density functional (DF) calculations obtain the correct ferromagnetic ground state of Fe. We had in the past demonstrated with the help of correlation calculations on 5 band Hubbard Hamiltonians that this is in part due to a chance compensation of big errors in the handling of local interactions. DMFT-calculations on similar models have shown that the biggest apparent DF-deficiency, the computed transition temperature, can be only partially improved, namely from 3500K to 2000K.

Recent ab-initio correlation calculations by the Local Ansatz falsify the underlying rigid band hypothesis in both approaches. While the non magnetic DF-results are the appropriate basis for the magnetic ground state, they fail for the non magnetic state itself. Here, not fully screened non local exchange contributions play a big role. The exact charge distribution is different, and the density of state is strongly modified, with n(EF) less than half the one of the DF-case. This causes an electronic first order phase transition. Also the resulting energy-bands differ. In contrast to the DF-results, these explain temperature dependent angular resolved photoemission experiments (Kirschner et al., PRL 53, 612 (1984)).

MM 20.2 Tue 10:30 H 0111

Transport through realistic junctions: Beyond DFT — •Frank Freimuth[1], Daniel Wortmann[1], Yuriy Mokrousov[2], and Stefan Blügel[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany — [2]Institut für Angewandte Physik, Universität Hamburg

DFT-based *ab initio* methods have become the standard tools for the investigation of materials' properties. However, the applicability of this method to electronic transport calculations is limited by the difficulties of describing excited states by ground state DFT. In this talk, we give an outline of how the local part of the Coulomb interaction may be taken into account via the self-energy in calculations describing electronic transport. Wannier functions constructed from the DFT Bloch states of the interface provide a localized set of basis functions adequate for the calculation of correlation effects using many-body techniques formulated for lattice systems. Our electronic transport method is based on the embedding technique, which provides a tool to calculate the Green function of the interface region of planar junctions suitable for application within *ab initio* studies of electronic transport. Our implementation of the embedding technique uses the full-potential linearized augmented plane-wave (FLAPW) method which does not make any approximations to the potential.

MM 20.3 Tue 10:45 H 0111

Fermiology of Cuprates and Non-Fermi Liquid Metallic Phases. — •Mukul Laad, Liviu Hozoi, and Peter Fulde — Max-Planck Institut fuer Physik komplexer Systeme, 38 Noethnitzer Strasse, 01187 Dresden, Germany

In the first step, we employ ab-initio wave-function based quantum chemical calculations to extract the effective hoppings for one hole/electron doped into a CuO2 plane. Strong, anisotropic, short-range spin correlations are found to drastically modify (bare) density-functional estimates of the hoppings. Remarkably, our results describe the detailed dispersion of the Zhang-Rice-like band (hole doping) as well as the unique evolution of both, hole- and electron-doped cuprates with quantitative accuracy. We discuss the implications of our findings

for many, Fermi surface based, physical responses and their evolution in cuprates as a function of doping.

In the second step, we build upon these results to study the dynamical correlations in cuprates by incorporating these results in a new cluster dynamical mean field approximation. The physical mechanisms underlying the emergence of the unique non-Fermi liquid metallic phase(s) in cuprates will be detailed, and several response functions will be described in relation to experiments.

MM 20.4 Tue 11:00 H 0111

Quantum-chemical approach to cohesive properties of metals: Anomalous behaviour of Be. — •Elena Voloshina[1], Beate Paulus[2], and Hermann Stoll[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, D-14195 Berlin — [3]Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart

Calculations based upon the incremental scheme [1], i.e. an expansion of the total correlation energy in terms of one-body, two-body and higher-order contributions, have been performed on a variety of solids with band gaps [2]. Metals require a special treatment. Via an embedding scheme, we can force localization in metallic-like model systems and can mimic the metallic band structure within finite fragments of the solid [3]. This allows for a gradual delocalization towards the infinite crystal within the incremental scheme. Up to now we successfully applied the method to magnesium [4] and group 12 elements [5,6] where in all cases the ground-state properties agree very well with experiment.The beryllium crystal has the same hcp structure as Mg; the atoms are characterized by closed ns^2 shells. At the same time Mg is almost free-electron-like whereas Be, although in general metallic, shows a lower density of states of almost entirely p character at the Fermi energy; that is the reason for the anomalous behavior of Be compared with other group 2 and 12 metals.

[1] PRB 46, 6700 (1992).
[2] Phys. Rep. 428, 1 (2006).
[3] JCP 126, 134115 (2006).
[4] PRB 75, 245117 (2007).
[5] PRB 74, 094102 (2006).
[6] PRB (in press).

MM 20.5 Tue 11:15 H 0111

Does magnesium-like zinc in a nearly ideal hcp form exist? — Nicola Gaston[1], •Beate Paulus[2], Ulrich Wedig[3], and Martin Jansen[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Zinc crystallises in the hcp structure, but with an anomalously large c/a ratio, indicating a strong distortion away from ideal packing. Density functional calculations of zinc fail to describe the unusual hcp structure of this material [1]. We perform a wavefunction-based correlation treatment on top of periodic Hartree-Fock calculations. This treatment corresponds to a many-body expansion of the correlation energy of the extended system in terms of localized orbital groups (method of increments)[2]. The Hartree-Fock treatment yields no binding and no equilibrium geometry for zinc. The binding of the ground-state structure is fully described by electronic correlations. Our values of the cohesive energy agree within 5% with the experimental value and within 2% for the lattice parameters. These calculations indicate additionally a local miminum of the potential energy surface for a c/a ratio which is almost ideally close-packed as in magnesium.

[1] B. Paulus, K. Rosciszewski, P. Sony, U. Wedig and M. Jansen Phys. Rev. B 75, 205123 (2007).
[2] N. Gaston and B. Paulus, Phys. Rev. B in press (2007)

MM 21: Quasicrystals

Time: Tuesday 11:45–13:00 Location: H 0111

MM 21.1 Tue 11:45 H 0111

The (010) Surface of the T-Al3(Mn,Pd) Complex Metallic Alloy — •Thalia Deniozou[1], Rafik Addou[1], Marc Heggen[2], Michael Feuerbacher[2], Oliver Gröning[3], Vincent Fournée[1], Julian Ledieu[1], and Jean-Marie Dubois[1] — [1]1LSG2M, UMR 7584 CNRS-INPL Ecole des Mines, F-54042 Nancy, France — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]3EMPA, Materials Science and Technology, Nanotech at Surfaces, Feuerwerkerstraße 39, CH-3602 Thun, Schweiz

The discovery of quasicrystals modified the basic concept of solid state physics, as they lack periodicity but still have long-range order and forbidden rotational symmetries. There is currently a broad interest in related systems, called complex metallic alloys, presenting a similar local order but recovering periodicity, though on a large scale compared to regular crystals. The orthorhombic phase T-Al3(Mn,Pd) is an example of such large unit cell crystal, approximant of the decagonal Al-Mn-Pd quasicrystal. Here we report the first study of the (010) surface of the T-Al3(Mn,Pd) phase, using scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED). The surface is prepared by sputtering and annealing to 900 K. The characteristic pseudo-decagonal symmetry and the orthorhombic unit mesh of the (010) T-Al3(Mn,Pd) surface could be observed with LEED. STM images reveal flat terraces separated by a unique step height (6.3 +0.3 Å). High-resolution images show a pattern of pentagonal chains characteristic of the bulk structure. We found that the contrast in STM images strongly depends on the bias voltage.

MM 21.2 Tue 12:00 H 0111

Are the Al atoms correctly placed in the models of i-AlPdMn and i-AlCuFe? — •Zorka Papadopolos[1], Oliver Gröning[2], and Roland Widmer[2] — [1]Institut für Theoretische Physik, Univ. Tübingen, Germany — [2]Material Science and Technology, EMPA, Thun, Switzerland

The model $\mathcal{M}(\mathcal{T}^{*(2F)})$ [1], as a model of atomic positions describes $Al_{70}Pd_{21}Mn_9$ and $Al_{62}Cu_{25.5}Fe_{12.5}$ [2]. The model is based on the diffraction results [3,4]. In the model we study the bulk terminations as defined in [5], through a generalisation of the Bravais' rule to the quasicrystals. Assuming the model independent results of LEIS (low energy ion scattering) [6], from the STM (scanning tunnelling microscopy) simulations [7] on the 5fold surface, compared to the real images of i-AlPdMn, we conclude that either the Al atoms are not correctly placed in the model, or the shape of atomic surfaces, i.e. the model of atomic positions itself must be changed.

[1] http://www.quasi.iastate.edu/Structure%20Dbase%20Info.html
[2] V. Elser, *Philos. Mag. B* **73**, (1996) 641.
[3] M.de Boissieu et al., *J. Phys.: Condens. Matter* **6**, (1994) 10725.
[4] A. Katz et al., in *Proc. of the 5th Int. Conf. on Quasicrystals*, ed. C. Janot et al., (World Scientific, Singapore, 1995) p. 164.
[5] Z. Papadopolos and G. Kasner, *Phys. Rev. B* **72** (2005) 094206.
[6] R. Bastasz et al., *Philos. Mag.* **86**, (2006) 855.
[7] J. Tersoff and D.R. Haman, *Phys. Rev. B* **31**, (1985) 805.

MM 21.3 Tue 12:15 H 0111

Observation of Archimedean-Like Tiling Structures on Decagonal Quasicrystalline Structures — •Jules Mikhael, Laurent Helden, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany.

Spontaneous formation of quasicrystals is typically only observed in rather complex metal alloys, for instance i-AlPdMn or d-AlNiCo, and strongly depends on the specific chemical composition. One way for forming monoatomic quasicrystalline structures is to use the surface of the quasicrystals as templates for adsorbed monolayers. Here we report a real space investigation of the phase behavior of micron-sized colloidal particles adsorbed onto a quasicrystalline decagonal substrate created by interfering five laser beams. An intermediate remarkably stable phase is found revealing likewise crystalline and quasicrystalline characteristics. It can be described as a Fibonacci sequence of periodic (3.3.3.4.4) Archimedean tiling segments. This result opens a route to identify the primordial parameters for the formation of pseudomorphic monoatomic quasicrystals.

MM 21.4 Tue 12:30 H 0111

Dominant motion vs. localization in quasiperiodic chains

— •Klaus Morawetz[1,2] and Michael Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Chains of coupled clusters arranged in a quasiperiodic sequence are analyzed with respect to the dynamics of wave packets. The recurrence probability is shown to show characteristic plateaus described by an interplay of localization and dominant motion. A three-mode model is developed which allows to understand the features of the recurrence probability as well as of the time-dependent width of the wave packets. The relation to waiting probabilities and anomalous diffusion is worked out. The consequences for the transmission coefficient realizable in experiments by sequences of quasiperiodic chains are discussed and the generalizations towards two-dimensional tilings are presented.

MM 21.5 Tue 12:45 H 0111

Phase behavior of colloidal particles on a 2D quasicrystalline substrate — •Michael Schmiedeberg and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

By using Monte-Carlo simulations, we study charged-stabilized colloidal particles in a two-dimensional decagonal potential and calculate their phase diagram as a function of the particle density and the strength of the substrate potential, which in experiments is realized by interfering laser beams.

As one expects, we find a triangular to liquid phase transition for small laser intensities and a ten-fold symmetric quasicrystalline phase for high potential strengths. For intermediate intensities, however, where the colloidal ordering is influenced by both the colloidal interaction and the substrate potential, we identify a series of interesting phases: For systems with low densities, where the number of colloidal particles is less than the number of potential minima, there is a quasicrystalline phase which exhibits bond orientations in 20 different directions. When the number of colloids exceeds the occurence of minima, we usually find a solid phase without any bond-orientational order. However, for certain densities the system locks into a highly ordered phase that is close to an Archimedean tiling.

MM 22: HV Paxton

Time: Tuesday 14:00–14:30 Location: H 1058

Invited Talk MM 22.1 Tue 14:00 H 1058

Grain boundary embrittlement and cohesion enhancement in copper — •Anthony Paxton[1], Alexander Lozovoi[1], Rainer Schweinfest[2], and Michael Finnis[3] — [1]Atomistic Simulation Centre, Queen's University Belfast, BT7 1NN, UK — [2]Science+Computing ag, Hagellocher Weg 71-5, 720270 Tübingen, Germany — [3]Imperial College London, Exhibition Road, London SW7 2AZ, UK

There has been a long standing debate surrounding the *mechanism* of grain boundary embrittlement and cohesion enhancement in metals. Embrittlement can lead to catastrophic failure such as happened in the Hinkley Point disaster, or indeed in the case of the Titanic! This kind of embrittlement is caused by segregation of low solubility impurities to grain boundaries. While the accepted wisdom is that this is a phenomenon driven by *electronic* or *chemical* factors, using language such as *charge transfer* and *electronegativity difference*; we believe that in copper, at least, both cohesion enhancement and reduction are caused by a simple *size effect*. We have developed a theory that allows us to separate unambiguously, if not uniquely, chemical and structural factors. We have studied a large number of solutes in copper using first principles atomistic simulation to support this argument, and the results of these calculations will be presented here

MM 23: Poster session

Time: Tuesday 14:45–18:00 Location: Poster B

MM 23.1 Tue 14:45 Poster B

Nanotomography of Biomaterials — •Stephanie Röper[1], Christian Zeitz[2], Christian Dietz[1], Nadine Drechsel[1], Anke Bernstein[3], Nicolaus Rehse[1], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken — [3]Experimentelle Orthopädie, Martin-Luther-Universität Halle-Wittenberg, D-06097 Halle/Saale

Biomaterials such as bone and teeth are nanocomposites of proteins and minerals. At the molecular length scale these materials have a stiff inorganic component (hydroxylapatite) that reinforces the soft organic matrix (type I collagen) through a recurring structural motif. To gather information of the nanometer scaled structure of these materials we use nanotomography. For this scanning probe microscopy (SPM) based method the specimen is ablated layer-by-layer by wet chemical etching and imaged with tapping mode SPM after each etching step. In our experiments we focus on cortical human bone (embedded and native) and human teeth. The stepwise etching is done in-situ in the SPM with an automated setup. We will present our latest volume images of human bone and teeth and discuss new concepts for adjusting the imaging parameters to maintain a good imaging quality.

MM 23.2 Tue 14:45 Poster B

Neutron Reflectometry Studies on Self-diffusion in Nano-Crystalline Fe Films: First Results — •Sujoy Chakravarty[1], Michael Horisberger[2], Thomas Gutberlet[2], Jochen Stahn[2], and Harald Schmidt[1] — [1]Institut für Metallurgie, AG Materialphysik, TU Clausthal, Germany — [2]Laboratorium für Neutronenstreuung, ETH Zürich & PSI, Villigen, Switzerland

Nano-crystalline metals show in comparison to their coarse grained counterparts improved mechanical properties like high hardness and fracture toughness and also interesting magnetic properties. At low temperatures mechanical deformation (grain boundary creep, grain boundary sliding), grain growth, and also thermal stability are essentially controlled or influenced by self-diffusion. For an understanding of these processes close to room temperature, we carried out self-diffusion measurements on nanocrystalline Fe films using neutron reflectometry. This method enables to determine extremely low diffusivities down to 10ˆ-25 mˆ2/s and also extremely small diffusion lengths < 1 nm, not possible with conventional methods. For diffusion studies, isotopic multilayers of the form Si(substrate)/[57-Fe(5 nm)/nat-Fe(10 nm)]x10 were deposited by using magnetron sputtering. The multilayers were annealed in the temperature range between 473 and 673K for different periods of time and neutron reflectivity has been measured in-situ. Further, structural characterization has been done by grazing incidence X-ray diffractometry, Moessbauer spectroscopy, atomic force microscopy, and electron microscopy. First results are presented and are discussed in the framework of grain boundary diffusion in the type C regime.

MM 23.3 Tue 14:45 Poster B

Nitrogen Diffusion in Amorphous Silicon (Carbo)Nitride Probed by Neutron Reflectometry — •Erwin Hüger[1], Thomas Gutberlet[2], Jochen Stahn[2], Michael Bruns[3], and Harald Schmidt[1] — [1]Institut für Metallurgie, AG Materialphysik, TU Clausthal, Germany — [2]Laboratorium für Neutronstreuung, ETH Zuerich & PSI, Villigen, Switzerland — [3]Institut für Materialforschung III, Forschungszentrum Karlsruhe GmbH, Germany

Covalently bound amorphous solids are distinguished by extremely low self-diffusivities, which necessitates the detection of extremely short diffusion lengths in order to prevent an overlapping of crystallization and diffusion processes during annealing. We present nitrogen diffusion studies on amorphous SiN_x and SiC_xN_y materials, which were carried out by neutron reflectometry on isotope heterostructures. Here, a se-

quence of 14-N and 15-N enriched layers are deposited by magnetron sputtering on silicon substrates. Due to the different coherent neutron scattering lengths of 14-N (9.37 fm) and 15-N (6.44 fm) a scattering contrast for neutrons occurs between chemically identical layers. Self-diffusivities are determined from the modification of the reflectivity due to interdiffusion of the two nitrogen isotopes after annealing at elevated temperatures. We present a systematic study on samples with 3, 5, 12 and 40 single layers and demonstrate that it is possible to detect miniumum diffusion lengths of 0.7 nm and self-diffusivities of $5x10^{-25}m^2/s$. The temperature and annealing time dependence of the diffusivities is analyzed and explained in the framework of structural relaxation processes.

MM 23.4 Tue 14:45 Poster B

Exciton formation in graphene bilayer — •Raoul Dillenschneider — University of Augsburg, Germany

Graphene, layers of two-dimensional honeycomb-array of carbon atoms, has attracted much interest these last few years due to its recent experimental accessibility and a wide variety of interesting properties. As the engineering application of the graphene layers attracts increasing significance, we need to explore, experimentally and theoretically, ways to enrich graphene's electrical properties and to control them. One way to achieve some control over the electrical properties is to change the number of layers and/or the bias applied across the layers.

The bias can also potentially control the formation of excitons. Since the applied bias leads to the charge imbalance in the two layers, it is natural to suspect that the Coulomb attraction of the excess electrons and holes on opposite layers would lead to an exciton instability

We consider the possibility of an excitonic instability for biased graphene bilayer in the framework of Hartree-Fock theory.

MM 23.5 Tue 14:45 Poster B

Soft absorption edges studied with hard x rays — •Henning Sternemann[1], Christian Sternemann[1], John S. Tse[2], Juha A. Soininen[3], Yong Q. Cai[4], Serge Desgreniers[5], Timothy T. Fister[6], Nozomu Hiraoka[4], Achim Hohl[7], Andreas Schacht[1], Gerald T. Seidler[6], György Vankó[8,9], Simo Huotari[8], Keijo Hämäläinen[3], and Metin Tolan[1] — [1]Fakultät Physik / DELTA, TU Dortmund, Germany — [2]Dept. Phys. & Engn. Phys., U Saskatchewan, Canada — [3]Div. X-ray Phys., Dept. Phys. Sci., U Helsinki, Finland — [4]NSRRC, Hsinchu, Taiwan — [5]Dept. Phys., U Ottawa, Canada — [6]Phys. Dept, U Washington, USA — [7]Inst. Mat. Sci., TU Darmstadt, Germany — [8]ESRF, Grenoble, France — [9]KFKI, Budapest, Hungary

Non-resonant inelastic x-ray scattering is a powerful tool to access shallow absorption edges using hard x-rays. This allows the study of low energy transitions under conditions which do not permit electrons and soft x rays as a probe. We present a variety of non-resonant inelastic x-ray scattering measurements of Si based compounds. Applications range from L-edge studies of elemental Si [1] and bulk amorphous Si monoxide [2] to the study of giant dipole resonances of Ba and I endohedrally intercalated in complex silicon networks. The experimental results are compared to calculations employing a real-space multiple-scattering approach [3]. Implications on the study of high-pressure induced phase transitions will be emphasized.

[1] H. Sternemann *et al.*, Phys. Rev. B **75**, 075118 (2007). [2] C. Sternemann *et al.*, J. Phys. Chem. Solids **66**, 2277 (2005). [3] J.A. Soininen *et al.*, Phys. Rev. B **72**, 045136 (2005).

MM 23.6 Tue 14:45 Poster B

Stability, electronic and magnetic properties of iron oxyhydroxides under high pressure: Insights from first principles — •Katrin Otte[1], Rossitza Pentcheva[1], and Jim Rustad[2] — [1]Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — [2]Department of Geology, UC Davis

Iron oxyhydroxides (FeOOH) play an important role in nature and technology, e.g. in binding heavy metals. The high pressure behavior of water containing minerals is important for understanding the processes in the Earth's crust and lower mantle. Using density functional theory (DFT), we investigate the structural, electronic and magnetic properties of the iron oxyhydroxide-polymorphs (α-, β-, γ- and *hp*-FeOOH) under high pressures. We find that under ambient conditions goethite (α) is the lowest energy phase, while at high pressures the *hp*-phase becomes more favorable. The relative stability of the different phases follows the trend obtained from recent calorimetric measurements [1]. Bond lengths are in a good agreement with available experimental data. While in the ground state Fe^{3+}-ions are coupled antiferromagnetically, at high pressures a transition to a ferromagnetic alignment takes place in *hp*-FeOOH. At ambient conditions all AFM phases are insulating within the generalized gradient approximation (GGA). However, a substantial improvement of the size of the band gap is achieved by including electronic correlations within the LDA+U method.

[1] C. Laberty and A. Navrotsky, Geochimica et Cosmochimica Acta 62, 2905-2913 (1998)

MM 23.7 Tue 14:45 Poster B

Investigation of Electronic Transport Mechanisms in Phase Change Materials — •Jennifer Luckas, Martin Salinga, Carl Schlockermann, Andreas Kaldenbach, Ursula Nellen, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The non-linearity of the electrical conductivity in the amorphous phase not only states to be the oldest of all puzzles in the field of phase change materials starting with Ovshinsky's discoveries in the 1960s, but also remains likely to be the most controversial one to this date. The most prominent effect in this context is the so-called threshold switching in the amorphous phase describing a sudden break down of resistivity in the presence of a critical electric field. Besides its scientific importance this effect is crucial for the currently most promising application of phase change alloys, i.e. electric memory (PCRAM).

Several theories about electronic transport of this class of materials have been proposed in the last decades, but there is still a lack of quantitative experimental data to validate or disprove them. To fill this gap in this work the mobility of the charge carriers is studied for some representative phase change materials. The dependence of the mobility both on temperature and on the electric field is investigated and compared with existing theories. From this comparison insight into the mechanism of charge carrier transport is obtained.

MM 23.8 Tue 14:45 Poster B

High Kinetic Energy Photoelectron Spectroscopy Study of the Ni 1s Core Level and Satellite Structure — •Mihaela Gorgoi[1], Svante Svensson[2], Olof Karis[2], Jan Rusz[2], Peter Oppeneer[2], Franz Schäfers[1], Walter Braun[1], Nils Martensson[2], and Wolfgang Eberhardt[1] — [1]BESSY GmbH, Berlin, Germany — [2]Uppsala University, Uppsala, Sweden

The Ni 2p level and its satellite structure have been studied since many years and the mechanisms behind this structure have been addressed in a large number of reports [1, 2 and references within]. In contrast, there is not a modern photoelectron spectrum of Ni 1s and the corresponding satellite structure. Using the HIKE facility at beam-line KMC1 at BESSY we have studied this core level using excitation energies from 9 keV to 12 keV. Our findings show that the satellite *main line energy distance decreases for the Ni 1s level in comparison to the Ni 2p case. Our finding has important implications for the existing theoretical explanations of the classical Ni satellite problem and requires a revision of current models.

[1] A.P. Grosvenor, M.C. Biesinger, R.St.C. Smart, N.S. McIntyre, Surface Science 600 (2006) 1771.

[2] A. Bosch, H. Feil, G.A. Sawatzky, N. Mårtensson, Solid State Communications 41 (1982) 355.

MM 23.9 Tue 14:45 Poster B

The importance of cluster-distortions in the tetrahedral cluster compounds: Ab initio investigations — Martin Sieberer, Stefan Turnovszky, Peter Mohn, and •Josef Redinger — Center for Computational Materials Science, Vienna University of Technology, Vienna, Austria

We study the electronic and structural properties of selected representatives of the so-called Molybdenum cluster compounds such as GaM_4X_8 with M=Mo as a group VIB element and V, Nb, Ta as a group VB element. X denotes either S or Se. These compounds are known to exhibit semiconducting behavior in the electrical resistivity, caused by hopping of electrons between well-separated metal clusters. The large separation of the tetrahedral metal (M_4) clusters is believed to be the origin of strong correlations. We show that recent calculations neglected an important type of structural distortions, namely those happening only within the M_4 unit upon a fixed angle $\phi = 60^o$ of the trigonal (fcc-like) cell. These internal distortions gain a significant amount of energy compared to the cubic cell and they are - to our knowledge - almost undetectable within powder x-ray diffraction. However, they strongly influence the band-structure by opening up a gap at the Fermi-energy, which puts into question whether all

compounds of this family are really called Mott insulators as stated elsewhere. In particular ferromagnetic $GaMo_4S_8$ and GaV_4S_8 are well described within DFT. Only the Nb and Ta-based representatives require a large effort due to the lack of magnetic long range order caused by frustrated AF M-M interactions.

MM 23.10 Tue 14:45 Poster B

Critical Packing Fraction in Multicomponent, Glass Forming Metallic Liquids — •Suresh M. Chathoth, Bernd Damaschke, and Konrad Samwer — I. Physikalisches Institut,Friedrich-Hund-Platz 1,37077 Goettingen,Germany

Glass forming Ni59.5Nb40.5 and Ni60Nb34.8Sn5.2 have been investigated in their equilibrium liquid by quasielastic neutron scattering. These liquids exhibit extraordinary high packing fraction[1]. Structural relaxation shows stretching in time and extent of stretching depends on the temperature of the liquid. The self-diffusivity decreases about two orders of magnitude within 360 K. From the beta-relaxation, tau-scaling analysis of self-diffusion and mean relaxation times of the alpha-process the critical packing fraction of these liquids have been derived. Our results provide, for the first time, an experimentally observed value for the critical packing fraction in the glass forming metallic liquids and is in good agreement with mode-coupling theory prediction[2].

We gratefully acknowledge the financial support from SFB 602 TP B8 and DLR under grant No. 50WM0541.

1.S. Mukherjee, Z. Zhou, W. L. Johnson, and W. K. Rhim, J. Non-Cryst. Solid 337, 21 (2004).

2.W. Götze, J. Phys: Condens. Matter 2, 8485 (1990).

MM 23.11 Tue 14:45 Poster B

Temperature dependence of elastic constants for the metallic glass $Pd_{40}Ni_{40}P_{20}$ — •Thomas Koeppe, Dennis Bedorf, and Konrad Samwer — 1. Physikalisches Institut Universität Göttingen, Germany

We have measured the elastic constants of bulk amorphous $Pd_{40}Ni_{40}P_{20}$ in the temperature range from 2 K to 300 K. The measuring technique was the ultrasonic pulse echo method with a frequency of 6 MHz. With decreasing temperature a linear increase of the elastic constants is found. At lower temperatures an increasing deviation from the straight line is observed. The Poisson ratio shows a linear decrease with decreasing temperature and deviates from that behavior at low temperatures also. This behavior is qualitatively the same as for single crystals and follows a $T^{\frac{3}{2}}$ - law down to our lowest temperature. The measured loss is very small at low temperatures and depends mainly on the bonding agent. So bulk amorphous metals are transparent for ultra sound at low temperatures. This work was supported financially by DFG, SFB 602 and Leibniz Programm.

MM 23.12 Tue 14:45 Poster B

Influence of a miscut of Y_2O_3-stabilized ZrO_2 single crystals on the formation of $La_2Zr_2O_7$ islands by a vapour-solid reaction — •Markus Andreas Schubert, Stephan Senz, and Dietrich Hesse — Max Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The $La_2Zr_2O_7$-forming solid state reaction between ZrO_2 and La_2O_3 is of significance in view of solid oxide fuel cells degrading during operation by a reaction of this type, if ZrO_2 is the solid electrolyte and if a La_2O_3-containing ternary oxide cathode is used. In model experiments, La_2O_3 vapour at 1200 °C directly reacts with an yttria-stabilized ZrO_2 single crystal (YSZ) forming $La_2Zr_2O_7$ (LZO) pyrochlore islands. Islands on YSZ(001) are square shaped and consist of four or eight slightly tilted domains. On YSZ(110), islands have a long edge along $[\bar{1}10]$ and a short edge along [001] and four tilted domains. The tilt of the islands is a consequence of the misfit accommodation mechanism for a vapour-solid reaction with a large positive misfit of +5 %.

New experiments were performed to investigate the influence of the miscut angle on the favoured formation of special domains. YSZ(001) and YSZ(110) single crystals with a miscut angle of 4° were used. For YSZ(001) substrates the surface was rotated around a [100] or [110] direction, respectively, and for YSZ(110) it was rotated around the $[\bar{1}10]$ or [001] direction. The relative orientation and morphology of the LZO islands were investigated by AFM, XRD and TEM.

MM 23.13 Tue 14:45 Poster B

PAC studies of Indium containing MAX phases — •Daniel Jürgens[1], Michael Uhrmacher[1], Hans Hofsäss[1], Jens Röder[2], Pawel Wodniecki[3], Agniszka Kulinska[3], and Michel Barsoum[4] — [1]II. Physik. Inst., Universität Göttingen, Germany — [2]Institut f. phys. Chemie, TU Braunschweig,Germany — [3]IFJPAN, 31 - 342 Krakow, Poland — [4]Dep. Mat. Science and Eng. Drexel Univ., Philadelphia, USA

Nanolaminated layered ternary carbides and nitrides, the so called MAX phases, have attracted great attention in recent time. By now over 50 compounds are known which feature a unique combination of the best attributes of both metals and high-performance ceramics. This class of materials for instance possesses good electrical and thermal conductivities as well as considerable damage tolerance and temperature oxidation resistance.

The method of perturbed angular correlation (PAC) with implanted ^{111}Indium as probe nuclei is successful in measuring the electric field gradient (EFG) of the A-site by using Indium containing MAX phases like Ti_2InC and Zr_2InC. These key-compounds provide a kind of fingerprint EFG that can be compared to other MAX phases which have no Indium in their structure. Special attention is payed to investigations of annealing parameters, thermal characteristics and behaviour under isostatic stresses.

MM 23.14 Tue 14:45 Poster B

Mechanical alloying and milling of Al-Mg alloys — •Mira Sakaliyska, Kumar Babu Surreddi, Sergio Scudino, and Jürgen Eckert — IFW Dresden, Institut für Komplexe Materialien, Postfach 270116, D-01171 Dresden, Germany

Solid solubility extension far beyond the room temperature equilibrium value was achieved by mechanical alloying of elemental powder mixtures for the binary Al-Mg system in the range of 10 - 50 at.% Mg. The Al(Mg) solid solutions are metastable and transform into the equilibrium phases during heating. No indication for the formation of the equilibrium phases (beta-Al3Mg2 and gamma-Al12Mg17) during milling was detected. Similar results can be achieved by mechanical milling of intermetallic compounds. For example, for Al60Mg40 mechanical alloying and milling yield the same metastable supersatured solid solution as end product. Upon heating, the milled powders prepared from different starting materials display a complex behavior characterized by several exothermic events. At low temperatures, an increasing amount of Mg is rejected from the solid solution with increasing temperature. At higher temperature, a hexagonal phase with composition Al3Mg2, is formed. The subsequent exothermic events correspond to formation and growth of the equilibrium beta-Al3Mg2 phase. Finally, selected examples for the mechanical deformation behavior of consolidated samples are presented, revealing encouraging properties regarding the combination of high strength and good ductility at room temperature.

MM 23.15 Tue 14:45 Poster B

New DFT-Investigations of Vanadium Silicides — Mike Thieme and •Sibylle Gemming — Forschungszentrum Dresden-Rossendorf, POB 51 01 19, 01314 Dresden, Germany

Vanadium and silicon form several binary compounds; the most well characterized structures have the compositions V:Si= 3:1, 6:5, 5:3, 1:2. Density-functional band-structure calculations with a plane-wave basis for the valence electrons and norm-conserving pseudopotentials for the core-valence interaction have been carried out to investigate the structural properties and the phase stability for the experimentally known binary crystals. As the early transition metal silicides belong to the class of refractory materials, also the elastic properties were determined. It is furthermore shown that the electronic properties of the compounds depend on the composition.

MM 23.16 Tue 14:45 Poster B

The behaviour of different equations of state under pressure — •Claudia Loose[1], Jens Kortus[1], Marcus Schwarz[2], Edwin Kroke[2], and Gerhard Heide[3] — [1]TU-Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany — [2]TU-Bergakademie Freiberg, Institute for Mineralogy Brennhausgasse 14 09596 Freiberg, Germany — [3]TU-Bergakademie Freiberg, Institute for Anorganic Chemistry, Leipziger Straße 29, Germany

We studied the effect of different Pseudopotentials and Equations of state (EOS) on the calculation of elastic properties (Bulkmodulus K and pressure derivative of the bulkmodulus K') and V_0 at different pressure ranges. We also calculated transition pressures for the system ALN (wurtzite - rocksalt) and SiO_2 (low quarz - coesite - stishovite)

with respect to Pseudopotential and EOS. At low pressure all EOS gave similar elastic properties whereas encreasing pressure leads to a divergence of about 10% while still fitting the same data. The transition pressure on the other hand depends only on the choise of Pseudopotential (LDA/GGA)

MM 23.17 Tue 14:45 Poster B

Hybrid electrode of carbon aerogels and metal oxides for electrochemical capacitors — •Volker Lorrmann[1], Henning Lorrmann[1], Ingo Riedel[1], Gudrun Reichenauer[1], Matthias Wiener[1], Carsten Deibel[2], and Vladimir Dyakonov[1,2] — [1]Bavarian Center of Applied Energy Research (ZAE Bayern), Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg, Germany — [2]Lehrstuhl für Experimentelle Physik VI, Julius-Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg

Electrochemical capacitors (EC) fill the gap between conventional capacitors with high power but low energy density and batteries with high specific energy density but rather low power density. There are two types of EC: Double-layer supercapacitors, which store charges electrostatically in the electrochemical double-layer between electrolyte and high surface area electrodes of activated hard carbon. In pseudocapacitance supercapacitors the charge storage is of faradaic-nature, e.g. redox processes in metal oxides. We have blended the organic precursor of a synthetic activated hard carbon (carbon aerogel) with metal oxide particles to be used as electrode for EC. The aim is to combine the faradaic- and the double-layer capacitance of the metal oxide and carbon, respectively, to increase the achievable capacity of the electrode. The electrochemical properties of these composites were investigated with cycling voltammetry, charge/discharge cycling and impedance spectroscopy. Structural analysis was performed via scanning electron microscopy and X-ray diffraction.

MM 23.18 Tue 14:45 Poster B

The Imaging Beamline at PETRA III — •Astrid Haibel, Felix Beckmann, Julia Herzen, Thomas Dose, Sven Utcke, and Andreas Schreyer — GKSS Research Centre Geesthacht

Since 2007 the GKSS is responsible for construction and operation of the Imaging Beamline at the new synchrotron source PETRA III at DESY. Due to the high brillance (most brilliant X-ray source worldwide), the low emittance of 1nm rad (unrivaled for current storage rings at comparable high particle energies) and the high fraction of coherent photons also in the hard X-ray range an extremely intense and sharply focused X-ray light will be provided. This advantages of the beam fulfil excellently the qualifications for absorption, phase contrast or holo tomography, for nano tomography and for high speed or in situ tomography. The first user operation of the facility is planned in 2009.

The Imaging Beamline will be structured into two experimental stations for micro and for nano tomography. The X-ray energy will be tunable between 5 and 50 keV. In the micro tomography hutch the investigation of samples of some millimeters diameter in (sub)-micrometer resolution is planned. Here, fields of application encompass questions from materials science (e.g. analysis of pores, cracks, precipitations, phase transitions) as well as problems in the area of biology or medicine (e.g. structures of bones, tissues, teeth, plants).

The possibility to focus the X-ray beam into the nanometer range will be used for nano tomographic imaging. Therefore, a second hutch for two nano tomography setups is planned. For this setups spatial resolutions down below 100 nm are expected for micrometer sized samples.

MM 23.19 Tue 14:45 Poster B

Synchrotron radiation based microtomography (SRμCT) and neutron tomography (NCT) for materials science — •Felix Beckmann, Julia Herzen, Tilman Donath, Astrid Haibel, Thomas Dose, Jürgen Vollbrandt, Heinz-Werner Schmitz, Philipp Klaus Pranzas, and Andreas Schreyer — GKSS-Research Centre Geesthacht, Germany

The GKSS-Research Centre Geesthacht, Germany, is operating the user experiment for microtomography using synchrotron radiation at the storage ring DORIS 3 at DESY Hamburg. In the recents years the beamline W2 was rebuilt. The outstanding feature of this synchrotron radiation beamline HARWI II is the use of high energy X-rays from 20 to 250 keV for materials science experiments. The features for microtomography at HARWI II and new enhancements and applications using lower photon energies at the wiggler beamline BW2 will be presented. Furthermore at the research reactor FRG-1 the neutron radiography facility GENRA 3 was extended by a setup for neutron tomography. Results performing SRμCT at HARWI 2 and NCT at GENRA 3 will be presented. The combination of neutron and synchrotron radiation techniques will give new insight into the three-dimensional behavior of samples in materials science.

MM 23.20 Tue 14:45 Poster B

Forensic Science - Applications in Metal- and Material Physics — •Horst Katterwe — Kriminaltechnisches Insitut / BKA, 65173 Wiesbaden

Forensic science refers to the examination of scenes of crime, recovery of evidence, laboratory examinations, interpreting of findings and presentation of the conclusions reached for intelligence purposes or for use in court. The paper describes forensic scientific cases, which can be solved by methods of applied metal- and material physics. Items and substances are bullets, cartridges, tool marks, fractures of metals and polymers, manufacturers marks and serial number restoration. Experiments which are employed include marks analysis, mechanical testing and recovering of erased characters by using aspects of solid-state physics, chemistry and engineering. Marking processes (die stamping, engraving, laser beam) change the microstructure of the metal (grains, slip bands, dislocations)or in cases of polymers the macromolecules around the marking become oriented (decreasing of the entropy). Methods used to restore erased numbers - both destructive and non-destructive - are described. \newline Reference: Voss-de Haan. Katterwe, Simross "Physik in der Kriminaltechnik", Physik Journal 2 (2003) Nr.9, 35-41.

MM 23.21 Tue 14:45 Poster B

The SKF Windows Expert Simulation Software SimCarb 2006 for Carburizing Case Hardening of Steels: a High-Performance CAE Tool for Industrial Process Optimization — •Jürgen Gegner — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Although case hardening of steels has been technically applied for more than one century, regular variance comparison tests of state-of-the-art operations based on two-step boost-diffuse gas carburizing treatments for determining the accuracy level of process control show that the target parameters are not met reliably. Whereas, for instance, the carburization depth should lie within 0.1 mm around its desired value, in practice a three times higher discrepancy represents a good heat treatment result. Inadequate computer control of the process is caused by its high complexity. Critical quantities are, e.g., the composition-dependent diffusivity and the concentration-activity relationship of carbon in the specific steel. The prerequisite for successful process optimization is a powerful simulation tool. Fundamentals, menu-driven handling, and application of the SimCarb software are presented. Fick's law of diffusion is solved by an implicit FD scheme under real boundary conditions. Material properties are selectable from large reference lists or freely defined by the user. In- and output are visualized online on the screen. Simulations can be saved in a special format. ASCII data export is supported. By advanced analysis, strategy development, feasibility study, and realistic prediction, SimCarb 2006 allows for efficient quality, sustainability and profitability improvement of case hardening.

MM 23.22 Tue 14:45 Poster B

Residual stress analysis of aluminium welds with high energy synchrotron radiation at the HARWI II beamline — •Torben Fischer, René V. Martins, and Andreas Schreyer — GKSS research centre, Max-Planck-Str. 1, 21502 Geesthacht

In civil aircraft production advanced welding techniques, like laser beam welding or friction stir welding, are used to reduce weight and production costs. By the welding process residual stresses are introduced in the weld zone and the surrounding area. These stresses may depend on diverse factors and can have disadvantageous influence on the service performance of the weld. For strain scanning GKSS research centre built up the high energy materials science beamline HARWI II at HASYLAB. The use of high energetic photons from about 80keV - 120keV enables diffraction experiments in transmission geometry, which provides the information about the macroscopic stresses. A large sample-detector-distance ensures a high angular resolution for the peak position determination. The heavy load diffractometer allows making use of massive sample environments.

For example laser beam welded t- and butt-joints were investigated with high spatial resolution. The large grain size of the specimen makes the measurements with high spatial resolution more difficult due to the poor grain statistics. The influences of the gauge volume size and grain

statistics on the strain measurements were systematically investigated. For the t-joint configuration two dimensional stress maps were calculated from the data. For the near future an in-situ FSW experiment is planed to investigate the metallophysical processes during the welding.

MM 23.23 Tue 14:45 Poster B

Field-driven evolution of stripe domains in magnetic shape memory alloy films — Nikolay S. Kiselev[1,2], Igor E. Dragunov[2], Aristide T. Onisan[1], •Ulrich K. Rössler[1], and Alexei N. Bogdanov[1,2] — [1]IFW Dresden — [2]Donetsk Institute for Physics and Technology

A phenomenological approach is used to describe the redistribution of martensitic variants driven by an external magnetic field in ferromagnetic shape memory materials. Real samples of magnetic shape memory alloys as the Ni-Mn-Ga Heusler alloys contain complex systems of crystallographic and magnetic domains [1, 2]. Magnetic reversal in such system is characterized by particular effects including the existence of 180-degree magnetic domain structures within the twin variants and the rotation of magnetic moments within magnetic domains in case of relatively weak magnetic anisotropies [1]. An elementary model for these complicated systems is proposed by using the "one-to-one correspondence" between magnetic domains and martensite variants [3]. For this model, we calculate stability ranges and evolution of equilibrium and metastable stripe states [3] and isolated twin-variants in thin single-crystalline plates. We discuss the applicability of this model to describe nucleation and magnetization processes in real samples.

[1] Y. W. Lai et al., Appl. Phys. Lett. 90 (2007) 192504; [2] V. A. Chernenko et al., Acta Mater. 53 (2006) 5461. [3] N. S. Kiselev et al., Eur. Phys. J. Special Topics, to appear.

MM 23.24 Tue 14:45 Poster B

Dependency of magnetic domain structures on stress and field history in bulk NiMnGa — •Ryan Yiu Wai Lai, Jeffrey McCord, Rudolf Schaefer, and Ludwig Schultz — Leibniz-Institute for Solid State and Materials Research, P.O.Box 270116, Dresden D-01171, Germany

A study of the magnetic domain structure in bulk NiMnGa magnetic shape memory single crystals is presented. Polarization microscopy, using a magneto-optical indicator film technique, is employed to obtain the static magnetic domain patterns at all surfaces of bulk crystals. Different complexity of domain patterns is revealed with different twinning states (e.g. single variant state, two-variant state). The dependency of domain patterns with stress and field history is investigated. Domain models explaining the observations will be discussed in detail. Funding through the DFG priority program SPP1239 is gratefully acknowledged.

MM 23.25 Tue 14:45 Poster B

Micromechanics of thin films of elastomeric polypropylenes — •Mechthild Franke, Mario Zerson, Mario Jecke, Robert Magerle, and Nicolaus Rehse — Chemische Physik, TU Chemnitz, 09107 Chemnitz

Elastomeric polypropylene consists of lamellar crystals embedded in an amorphous matrix. The arrangement, distribution, and connectivity of these crystals are important factors which determine the mechanical properties of the polymer. Free standing, $\sim$1 μm thick films of different elastomeric polypropylenes are produced by dip coating the polymer solution on a NaCl crystal, floating the film onto water, and depositing it on a slotted silicon substrate. A stretching device, based on a piezoelectric drive, allows stretching the free standing film stepwise up to strains of 100%. The changes in shape, orientation, and morphology of crystalline regions are observed in situ with scanning force microscopy. Caused by the induced stress new lamellae crystallize; existing ones elongate or break into blocks. Furthermore, amorphous areas are stretched a lot more than crystalline ones. Volume images of thin films obtained with SFM based Nanotomography allow to explain some of the observed rearrangements of the microstructure.

MM 23.26 Tue 14:45 Poster B

Aktuelle Forschung an der Bonner Positronen Mikrosonde — •Sven-Martin Hühne, Marius Wirtz, Patrick Eich, Matz Haaks und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, D - 53115 Bonn

Die Bonner Positronen Mikrosonde (BPM) ist derzeit ein einzigartiges Messinstrument, das mit Hilfe der Positronenannihilation zerstörungsfrei die Defektdichte in Metallen und Halbleitern in hoher Ortsauflösung messen kann.

Die BPM bietet einen fein fokussierten Positronenstrahl mit einstellbarem Stahldurchmesser von 5 - 200 μm und ein integriertes Rasterelektronenmikroskop (REM). Dadurch ist es möglich mit der BPM mit hoher lateraler Auflösung Plastizität und Defektdichte in verschiedenen Materialien zu messen.

Aktuelle Forschungsschwerpunkte liegen in der Abbildung von Deformationszonen und Ermüdungsstrukturen. Des Weiteren werden die Ergebnisse der durch Positronenannihilation gemessenen Defektdichte mit den klassischen Methoden zur Bestimmung der Schädigung wie Röntgen-Beugung (Debye-Scherrer Methode) und Vickers-Härte Messungen verglichen. Die in den Abbildungen erkennbare Entwicklung der Fehlstellendichte wird zur Vorhersage des Materialversagens in der Deformationszone herangezogen. Es zeigt sich, dass die Untersuchung der Defektdichte zu einer präzisen Schadensvorhersage führt, wie sich an aktuellen Messungen von Ermüdungsstrukturen an ferritischem und austenistischem Stahl veranschaulicht hat.

MM 23.27 Tue 14:45 Poster B

Introduction of Slip System Resolved Statistical Work Hardening Model — •Denis Novokshanov and Volker Mohles — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen Kopernikusstr. 14, D-52074 Aachen, Germany

A slip system resolved statistical work hardening model for single crystals has been developed. It is based on the dislocation density-based work hardening model 3IVM+, which in turn is an improved version of the 3IVM (three internal variables model) [1]. 3IVM+ predicts stress-strain curves for large ranges of temperature and strain rate. In the new model, the microstructure evolution of 3IVM+, i.e. the dislocation density evolution, is left unchanged. But the kinetic equation of state of 3IVM+ has been inverted: the new model considers the glide velocity of dislocations as a function of temperature and the external applied stress. This allows to consider each glide system individually by applying the corresponding Schmid factor in the stress projection. Hence all slip systems contribute to the overall deformation according to their intrinsic kinetics, which is defined by the crystal's orientation and the load axis. This leads tho realistic stress-strain curves and orientation changes for a single crystal. The model can be used as a replacement for 3IVM(+) in engineering applications of FEM. For polycrystals, the interaction between grains can be introduced in future by elastic stresses caused by differing rotations of adjacent grains.

1. F. Roters, D. Raabe, G. Gottstein, Acta Materiallia 48 (2000) 4181-4189

MM 23.28 Tue 14:45 Poster B

$Pd_{81}Si_{19}$-Metallic Nanoglasses with Enhanced Excess Volume — •Yue Zhang, Horst Hahn, and Herbert Gleiter — Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany

$Pd_{81}Si_{19}$ metallic nanoglasses were synthesized by inert gas condensation and in situ compaction. In this technique, amorphous nanoparticles, prepared by evaporation in an inert gas atmosphere, are collected and subsequently compacted using uniaxial pressures. During the compaction, surfaces are converted into internal interfaces and additional free volume is introduced into the amorphous structure. Wide angle X-ray diffraction and high resolution electron microscopy are employed to characterize the atomic structure. The excess volume fraction was calculated using classical free-volume theory from differential calorimetric scanning data. In order to have a comparison, glassy ribbons and bulk metallic glass rods with the same chemical composition were prepared using melt-spinning and B_2O_3 flux casting techniques, respectively. Comparing with these conventional metallic glasses, the $Pd_{81}Si_{19}$ nanoglasses exhibit an enhanced excess volume, resulting in modified properties.

MM 23.29 Tue 14:45 Poster B

The Grain Refinement in a Commercial Al-Mg-Sc-Zr Alloy during Hot ECAP and Subsequent Isothermal Rolling — •Olga Sukhopar[1], Oleg Sitdikov[2,3], Günter Gottstein[1], and Rustam Kaibyshev[4] — [1]Institute of Physical Metallurgy and Metal Physics, RWTH, Aachen 52074, Germany — [2]Institute for Metals Superplasticity Problems, Ufa 450001, Russia — [3]Department of Engineering Physics, Electronics and Technology, Nagoya Institute of Technology, Nagoya 466-855, Japan — [4]Belgorod State University, Belgorod 308034, Russia

Grain refinement taking place in a commercial Al-Mg-Sc-Zr alloy under equal channel angular pressing (ECAP) and subsequent isothermal rolling, which were carried out at a temperature of 325°C, was exam-

ined. With increase of strain the initial grains were highly elongated along the extrusion direction, and new fine grains formed along initial boundaries composing mantle region. Then new grains with size ˜ 1.5 μm were evolved in the grain interiors. During subsequent rolling the fraction of recrystallized grains increases. However, even after highest strains attained no full recrystallized structure was observed. Texture measurements have shown a randomly oriented structure. These results suggest that the dynamic evolution of new grains can be result from (sub)grains rotation, which leads to a rapid increase in misorientation of grain boundaries and to texture randomization. It was shown that progressive increase of misorientation of deformation induced boundaries (continuous dynamic recrystallization) is the main mechanism of submicrocrystalline grain formation.

MM 23.30 Tue 14:45 Poster B

zinc nano-cluster investigated by molecular dynamic simulations — •Stephan Braun, Frank Römer, and Thomas Kraska — Institute for Physical Chemistry, University Cologne, Germany

We perform molecular dynamics simulation with a recently developed new parameterisation of the embedded atom method (EAM) in order to investigate zinc nano-cluster. Nano-clusters exhibit differences in several properties compared to the bulk phase. In this context zinc is especially interesting because it is a hcp metal with a large deviation of the lattice axis ratio c/a to the ideal value corresponding to close packing. The clusters investigated here are obtained in prior particle formation simulations in a supersaturated vapour. The clusters are naturally grown including cluster-cluster collisions and sintering. Influences of the initial configuration to the resulting structures are not present. To control the temperature of the clusters we add argon as carrier gas which itself is coupled to a MD thermostat. We study the structure and morphology of the clusters for different temperatures and cluster sizes. Besides using the radial distribution function we employ the common neighbour analysis (CNA), which allows to determine details of the structural composition of the clusters. For this investigation we have developed CNA signatures especially for hcp-surfaces that are important for particle growth. We also analyse the thermal expansion and the equilibrium distance of the lattice constants for solid-like clusters.

MM 23.31 Tue 14:45 Poster B

Wassersorption in porösen Kohlenstoffen — •Philipp Eitelwein, Stephan Braxmeier und Gudrun Reichenauer — Bayerisches Zentrum für Angewandte Energieforschung, Am Hubland, 97074 Würzburg

Wird Wasserdampf in porösen Kohlenstoffen adsorbiert, so lässt sich eine makroskopische Längenänderung der Probe feststellen. Diese Änderung hängt vom relativen Druck des umgebenden Wasserdampfs ab. Es zeigt sich außerdem, dass sich die Adsorption in Poren unterschiedlicher Größe unterschiedlich verhält, denn Mikroporen (Poren $<$ 2 nm) lassen sich über Adsorption aus der Gasphase vollständig befüllen, während dies bei Meso- und Makroporen nicht der Fall ist. Zum besseren Verständnis wurden systematische Untersuchungen an Kohlenstoff-Aerogelen als Modellmaterial durchgeführt. Diese synthetischen Kohlenstoffe besitzen sowohl Makro- oder Mesoporen als auch Mikroporen; beide Spezies können während der Synthese gezielt variiert werden. Mittels unterschiedlicher Methoden, wie Röntgenkleinwinkelstreuung an unterschiedlich stark befeuchteten Proben und Messung von Sorptionsisothermen bei gleichzeitiger Bestimmung der Probenlänge, wird der Einfluss der Porengrößen auf die Längenänderung der Probe bei Ad- und Desorption systematisch untersucht. Aus den Daten werden Rückschlüsse auf die mit der Sorption auf mikroskopischer Längenskala verknüpften Effekte gezogen.

MM 23.32 Tue 14:45 Poster B

Intershell conductance in multiwall carbon nanotubes — •Andreas Stetter, Christian Back, and Johann Vancea — Universität Regensburg, Institut für angewandte Physik

We have measured the current induced voltage drop along an individual mutiwall carbon nanotube (MWCNT) as a function of the distance to the current injecting electrode. For this purpose we used the scanning probe potentiometry combined with scanning electron microscopy.

For a MWCNT with an incomplete outer shell a sharp potential jump was observed at the end of the outer shell. The length dependence of the potential on the whole tube has been used to determine the intershell conductance of the MWCNT.

MM 23.33 Tue 14:45 Poster B

Fabrication of metallic nanowires and their hydrogen sorption — •Felix Schlenkrich, Sönke Schmidt, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Nanowire alignments of palladium and niobium have been produced by small angle sputtering onto facetted sapphire and sputter-eroded silicon, using the self shadowing effect of the facets and ripples, respectively. The achieved wire length is in the cm range (length of sample) and wire widths of 50nm and heights of 15nm were obtained. Island growth has been investigated, and the regimes of coalescence and fully covered wire morphology of the metallic stripes onto the facets and ripples were achieved. Wire characterisation and the behaviour of metal wires during the exposure in hydrogen atmosphere (surface modification) was investigated with STM and AFM, using Non-Contact mode and Contact mode. Resistivity measurements on palladium wire alignments during hydrogen loading were performed. The influence of hydride formation on the resistivity of the wires will be discussed.

MM 23.34 Tue 14:45 Poster B

Quantum conductance of copper nanowires — •Saeideh Mohammadzadeh[1], Davoud Pouladsaz[2], Reinhard Streiter[1], and Thomas Gessner[1] — [1]Zentrum für Mikrotechnologien, Technische Universität Chemnitz — [2]Institut für Physik, Technische Universität Chemnitz

Electronic transport properties of the Cu nanowires are studied using theoretical analysis based on non-equilibrium Green function's technique within the density functional tight-binding method. The systems, presented in this work, consist of Cu nanowires in various crystalline directions, coupled between semi-infinite copper electrodes. The current-voltage characteristics of the wires and charge density with non-equilibrium conditions are investigated as well.

MM 23.35 Tue 14:45 Poster B

Determination of lattice distortion in nanoparticles on strained substrates using molecular dynamics — Jian Zhou, •Srinivasa Saranu, and Ulrich Herr — Institut für Mikro- und Nanomaterialien, Universität Ulm, 89081 Ulm

Magnetoelastic anisotropies might provide a way to optimize the magnetic properties of nanoparticles. The experimental determination of strain in nanoparticles is often complicated by the low XRD intensities. We used the molecular dynamics simulation technique to determine the deformation of Co particles deposited on Ta or Cu substrates. Co particles of 4.5 nm diameter with fcc structure were built using a Wulff construction and subsequently deposited on the substrates with a kinetic energy of 0.1eV/atom. The structure and internal strain in the particles have been determined from simulated diffraction curves. In some cases we find a fcc-to-hcp phase transformation in the particles which turns out to be related to the impact energy and the interface structure between the particle and substrate. The analysis also shows that the landed particles are always tilted with respect to the substrate surface. The degree of tilt is associated with the shape of the Co Wulff polyhedron. We have also studied the deformation induced in the particles by a change of the lattice parameter of the substrate after the deposition. We find that only coherent or semicoherent interfaces can transfer strain from the substrate to the deposited Co particles effectively.

MM 23.36 Tue 14:45 Poster B

Anomalous small-angle x-ray scattering beamline B1 at HASYLAB, DESY — •Ulla Vainio[1], Günter Goerigk[2], and Rainer Gehrke[1] — [1]HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, Postfach 1913, D-52425 Jülich, Germany

Anomalous small-angle x-ray scattering (ASAXS) is a contrast variation technique used for studying the structure of complex materials which have coexisting inhomogeneities of different chemical composition. By measuring at different photon energies near an absorption edge of a certain chemical element contained in the sample, the small-angle scattering caused by the distribution of that element can be distinguished from other scattering contributions caused by other elements or by voids in the case of porosity. This is possible because the scattering factor of the considered element changes significantly near its absorption edge.

The dedicated instrument is optimized for this kind of measurement in terms of precision. The energy of the radiation can be tuned from

5 keV up to 35 keV and accurate x-ray absorption scans can be performed.

The beamline is located at a bending magnet at the DORIS storage ring. It was originally built by research centre Jülich in the 1980s and was upgraded in collaboration with HASYLAB in 2006 (G. Goerigk (2006) HASYLAB annual report, pp. 77 - 78) . Since July 2007 the beamline is operated by HASYLAB.

MM 23.37 Tue 14:45 Poster B

Stress impact on reactive diffusion in nano-structures of spherical symmetry — •Constantin Buzau Ene[1], Guido Schmitz[2], Carsten Nowak[1], Talaat Al-Kassab[1], and Reiner Kirchheim[1] — [1]Universität Göttingen, Institut für Materialphysik, Friedrich-Hund Platz 1, D-37077 Göttingen — [2]Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str.10, D-48149 Münster

Al/Cu/Al and Cu/Al/Cu triple layers with approximately 10 nm single layer thickness are deposited on curved substrates of 25 nm radius and investigated by atom probe tomography. The first reaction product is found after 5 min thermal treatment at 110°C. Surprisingly, the reaction rate depends significantly on the deposition sequence of the metals. Thus, the thickness of the product formed at the interfaces at which Cu is deposited on top of Al is approximately 1.5 to 2 times thicker than that of the opposite stacking sequence. This asymmetry may be explained by stress induced by excess volume of the reaction product. Due to the specific geometry, compressive and dilatational stress is produced on opposite sides of the product layer, even in the case of semi-coherent or incoherent interphase boundaries. The resulting stress gradient leads to additional driving force to the transport of vacancies which accelerates or decelerates the reaction rate in dependence on the stacking sequence of the layer material. By quantitative analysis, the level of induced stress can be quantified from the modified growth rates.

MM 23.38 Tue 14:45 Poster B

Charge separation between type II aligned closed packed CdTe and CdSe nanocrystals — •Dieter Gross, Andrei S. Susha, Thomas A. Klar, Andrey L. Rogach, and Jochen Feldmann — Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Germany

Combinations of CdTe and CdSe provide type II structures with the lowest excited energy state for electrons in CdSe and the lowest excited hole state in CdTe. This kind of energy level alignment facilitates the separation of photo-excited charge carriers in modern thin film solar cells. We have observed an efficient photoluminescence quenching and a reduced life time of the CdTe nanocrystal emission in hybrid structures made of colloidal CdTe and CdSe nanocrystals. These effects have been observed in both, layered structures created by a layer-by-layer technique and clustered assemblies in solution, providing both a controlled assembly with a short inter-particle distance (< 1 nm). We interpret this suppression of the CdTe emission to be due to spatial charge separation of the photo-excited electron-hole pairs.

MM 23.39 Tue 14:45 Poster B

Tailoring the diameter of nanowires by controlled anodic oxidation and its electrical properties — •Seid Jebril, Samia Essa, Mady Elbahri, and Rainer Adelung — Functional Nanomaterials, Institute for Material Science, CAU Kiel, Kaiserstr. 2, 24143 Kiel

Resizing the diameter of the already formed nanowire has been a great challenge to achieve for the last decades. Here, we show tailoring of a nanowire by using anodic oxidation. Anodic oxidation has been used for formation of core-shell structures, protective layers, decorative or functional properties, to cite some. The polycrystalline nanowire used in this experiment was made by a method similar to what we developed earlier [1, 2]. We studied the electrical properties of the nanowire during and after the process. As a result of this potential controlled anodic oxidation, the diameter of the nanowire gets smaller and smaller as the oxide grows. Therefore, the electrons encounter dominant surface and boundary scattering due to confinement. Hence, the electronic properties change completely.

[1] R. Adelung et. al., Nature Mater. 3, 375, (2004).
[2] M. Elbahri et al., Adv. Mater. 18, 1059 (2006).

MM 23.40 Tue 14:45 Poster B

Tailoring carbon nanotubes through predefined catalyst particles — •Christoph Schünemann, Franziska Schäffel, Mark H. Rümmeli, Christian Kramberger, Thomas Pichler, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Owing to their excellent mechanical and electronic properties, carbon nanotubes (CNTs) are promising candidates for the integration into nanoelectromechanical systems such as nanorelays and actuators or transistors. Effective control of the CNT growth, orientation and positioning is still considered a mayor challenge within the scientific community.

In order to reach this goal, we use nanoparticles which are prepared via inert gas condensation as predefined catalysts to grow CNTs in thermal CVD and plasma enhanced CVD. Besides utilizing commonly used transition metal catalysts such as Fe, Ni and Co, we demonstrate the CNT growth from binary alloy catalyst particles, e.g. FePt.

MM 23.41 Tue 14:45 Poster B

Electric field controlled metal-oxide transformation of metal nanowires — •Carsten Nowak[1], Guido Schmitz[2], and Reiner Kirchheim[1] — [1]Universität Göttingen, Institut für Materialphysik, D-37077 Göttingen — [2]Universität Münster, Institut für Materialphysik, D-48149 Münster

Under high electrostatic fields E, tip-shaped metal nanowires transform into the corresponding oxide at room temperature if a certain partial pressure p of water is present. A TEM investigation of this reaction was performed on nanowires of tungsten and aluminum as well as silicon.

The oxidation reaction starts at a critical field strength $E_c(p)$ of the order of 10^9 V/m and proceeds until a quasi stationary state is reached. The kinetics of the reaction is gas supply-limited for pressures below 10^{-3} mbar and proceeds with rates corresponding to a diffusion coefficient of the order of 10^{-15} m^2/s for a vapor pressure in the 10 mbar range, indicating driven diffusion.

Determination of the the electric field distribution inside the oxide using the finite element method and the results of current measurements during the oxidation reaction indicate that the critical step of the oxidation process is a surface reaction at the oxide-vapor interface. A quantitative model describing the observed $E_c(p)$ dependence is given.

MM 23.42 Tue 14:45 Poster B

Electronic transport properties of nanocomposite materials prepared by electron and ion beam induced deposition — •Christina Grimm, Dirk Klingenberger, Harald Drings, and Michael Huth — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany

A survey is given of the electronic transport properties of tungsten-based nanocomposite materials prepared with electron (EBID) or ion (IBID) beam induced deposition employing $W(CO)_6$ as precursor. The samples are analyzed in the normal state with regard to temperature-dependent electron correlation corrections to the Drude conductivity. A $\sqrt{T}$-dependence of the electrical conductivity was found for the first time in samples prepared by EBID. IBID samples with metal content approaching 50% show superconducting transitions at approx. 5 K. The properties of these samples are analyzed on the basis of the transport theory of Josephson-coupled networks. Finally, recent results on employing these materials for sensor applications are presented.

MM 23.43 Tue 14:45 Poster B

Lattice dynamics of ferromagnetic shape memory alloys from inelastic neutron scattering — •Tarik Mehaddene[1], Juergen Neuhaus[2], Winfried Petry[1,2], Klaudia Hradil[2,3], and Philippe Bourges[4] — [1]Physik-Department E13, Technische Universitaet Muenchen, D-85747 Garching, Germany — [2]Forschungsneutronenequelle Heinz Maier-Leibnitz, D-85747 Garching, Germany — [3]Institut fuer Physikalische Chemie, Georg-August-Universitaet, D-37077 Goettingen, Germany — [4]Laboratoire Leon Brillouin (LLB), CEA Saclay, F-91191 Gif sur Yvette Cedex, France

The tendency of shape memory alloys to undergo a martensitic transtion shows up in the anomalous phonon softening of particular phonon modes in their austenitic phase. We report on phonon measurements in both austenitic and martensitic phases of Ni-based alloys. We show that, contrary to NiMnSn, the anomalous softening of the TA_2[110] phonons in NiMnGa is strongly enhanced below the Curie temperature. The measurements revealed that low restoring forces against the shearing of the (111) atomic planes along [11-2] develop upon cooling. The vibrational spectra measured in two different martensitic phases of NiMnGa, namely the tetragonal 5M and

the orthorhombic 7M structures, revealed fundamental differences. A dispersive low-energy excitation develops from the elastic modulation peaks in the 5M structure and come into interaction with TA_2[110] phonon branch in the q-range 0.25-0.3 r.l.u where the latter shows a wiggle in the dispersion. No wiggle is seen in the TA_2[110] branch of the 7M structure. It shows a normal sinus-like dispersion curve.

MM 23.44 Tue 14:45 Poster B

Phase diagrams for the evolution of polydomain and polyvariant states in tetragonal ferromagnetic martensites — •Aristide T. Onisan[1], Nikolay S. Kiselev[1,2], Ulrich K. Rössler[1], and Alexei N. Bogdanov[1,2] — [1]IFW Dresden — [2]Donetsk Institute for Physics and Technology

A continuum model for equilibrium microstructures in ferromagnetic twinned martensites is developed [1] that couples micromagnetic domain theory with anisotropic crystal elasticity and is applicable for magnetic shape memory materials as the Ni-Mn-Ga Heusler alloys. The approach considers the twin variant redistribution in tetragonal martensites with no-slip condition at the twin boundaries, magnetic 180°-domain structures within twins, and the rotation of magnetization within domains due to finite magnetic anisotropies. For two-variant twinned single crystals, we calculate equilibrium phase diagrams, strain and magnetization curves under combined external magnetic fields and stresses within the thermodynamic phase theory approximation. The limitations of the phase-theory approximation are discussed. For three-variant twinned microstructures, we show that magnetic charges arise internally at the twin boundaries. [1] A.N. Bogdanov, A. DeSimone, S. Müller, U.K. Rößler, J. Magn. Magn. Mater. 261 (2003) 204. *Supported by DFG, SPP 1239 project A08.*

MM 23.45 Tue 14:45 Poster B

Correlated ferroelastic/ferromagnetic domain walls in ultrathin films: observations and physical description — •Catherine Jenkins[1,2], R Ramesh[1], and Gerhard Jakob[2] — [1]University of California, Berkeley — [2]Johannes Gutenberg-Universität Mainz

The magnetic shape memory (MSM) effect is when simultaneously occurring ferromagnetic and ferroelastic domain walls form a twin boundary system that is actuated in one of three ways: by a magnetic field, a mechanical stress, or heating. Thin films of MSM alloys are exciting candidates for research because of the many variables that can be efficiently explored in a single system, and are promising for technological development for their novel magnetic and electronic characteristics.

Theoretical predictions in the literature (1), along with a physical understanding of the processes involved (2) together suggest that the thermoelastic austenite to martensite phase transition that allows for the 'memory' can be explored with temperature-dependent atomic force microscopy, as we show experimentally in fairly thick films of another shape memory alloy, nickel titanium. The behaviour of ultrathin films is expected to be noticeably different due to strong epitaxial clamping effects. In this work the expected topographic behaviour of ultrathin shape memory alloys during a magnetically and thermally induced phase transition and evolution is described and preliminary measurements presented.

1. Bertram HN, Paul DI, J Appl. Phys., vol.82, no.5, 1997, p. 2439
2. S. J. Murray et al, J. Appl. Phys., vol. 87, No. 9, 2000, p. 5774

MM 23.46 Tue 14:45 Poster B

Laser ablation of aluminium — •Steffen Sonntag, Johannes Roth, Frank Gähler, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

We investigate femtosecond laser ablation of metals using a hybrid simulation scheme. Two equations are solved simultaneously: one for the electronic system, which accounts for laser energy absorption and heat conduction, the other for the dynamics of the lattice where the ablation process takes place. For the electron temperature a generalized heat conduction equation is solved by applying a finite difference scheme. For the lattice properties, e.g. pressure, density or temperature, we use common molecular dynamics. Energy transfer between the subsystems is allowed by introducing an electron-phonon coupling term. This combined treatment of the electronic and atomic systems is an extension of the well known two-temperature model [1].

Atomic scale images of the ablation process are shown. The dependence of ablation and melting depth on characteristic parameters, such as the pulse duration and the laser fluence is discussed.

[1] S.I. Anisimov, B.L. Kapeliovich and T.L. Perel'man: Sov. Phys. JETP 39, 375(1974)

MM 23.47 Tue 14:45 Poster B

Structural Properties of the Metastable State of Phase Change Materials Investigated by Synchrotron Radiation — •Philipp Merkelbach[1], Julia van Eijk[1], Carolin Braun[2], and Matthias Wuttig[1] — [1]I. Phys. Institut (IA), RWTH Aachen, 52056 Aachen — [2]Institut für Anorg. Chemie, CAU Kiel, 24098 Kiel

Phase change alloys are among the most promising materials for novel data storage devices. Since several years Phase Change Materials based on Ge-Sb-Te- alloys have been used in optical data storage solutions like rewriteable CDs and DVDs. Recently these alloys have been explored as potential candidates for fast nonvolatile electrical data storage devices in Phase Change Random Access Memory (PCRAM).

Besides attracting considerable interest from the commercial point of view phase change materials are very interesting also due to their remarkable physical properties. They have the ability to be reversibly switched within a few nanoseconds between the amorphous and the crystalline phase, while changing their physical properties such as optical reflectivity and electrical resistivity significantly. Even though the electronic properties show a drastical contrast such fast transitions can only be caused by small atomic rearrangements. This behavior calls for a deeper understanding of the structural properties of the alloys.

We have performed powder diffraction measurements of the crystal phase of various GeSbTe alloys, to determine the structural similarities and differences of several alloys. Understanding the crystal structure of phase change materials is a key to a deeper insight into the properties of these promising materials.

MM 23.48 Tue 14:45 Poster B

Crystallization kinetics of phase change materials — •Andreas Kaldenbach, Martin Salinga, Ursula Nellen, Carl Schlockermann, and Jennifer Luckas — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase Change RAM is one of the most promising technologies for future memory applications outperforming alternatives mainly by its extreme scalability besides its non-volatility. It is based on a so-called phase change material switching between its highly resistive amorphous and lowly resistive crystalline state. While phase change materials are already utilized in applications, their remarkable physical properties are not yet understood in all detail. Ironically its most characteristic property, the crystallization kinetics, still has not been determined experimentally beyond a quite limited temperature range around the glass transition temperature and slightly below the melting temperature respectively. The uncertainty about the crystallization behavior in the intermediate temperature regime has so far been coped with by applying existing theoretical equations for a continuous description of nucleation and growth. However, until now these theories have not yet been validated by experimental evidence for the mentioned class of materials. The lack of experimental data is mainly caused by the high crystallization speed of phase change materials being truly demanding in respect to both the heating rates and the detecting system of an experiment. Thus an optical setup is assembled to conduct measurements of the phase change utilizing a pulsed laser. Experimental results are compared with existing theories on crystallization.

MM 23.49 Tue 14:45 Poster B

Characterization of a FePd single crystal for sensor applications — •Christoph Bechtold[1], Andreas Gerber[1], Manfred Wuttig[2], Eckhard Quandt[3], Jeff McCord[4], Yiu Wai Lai[4], Jörg Buschbeck[4], Ludwig Schultz[4], Oleg Heczko[4], and Sebastian Fähler[4] — [1]Research Center caesar, Ludwig-Erhard-Allee 2, 53175 Bonn — [2]Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742 — [3]Christian-Albrechts-Universität zu Kiel, Chair for Inorganic Functional Materials, Kaiserstr. 2, 24143 Kiel — [4]IFW Dresden, P.O. Box 270166, 01171 Dresden

Magnetic shape memory (MSM) materials have received much attention in actuator applications due to their large strains and short response times. However, their potential as an alternative to conventional magnetostrictors in sensor systems has not been studied so far. A FePd single crystal was characterized by EDX, VSM, DSC and temperature dependent XRD analysis. The magnetic field induced strain under different compressive loads was studied at temperatures ranging from 0 to -40°C and magnetic field induced actuation and twin boundary movement were confirmed and quantified by temperature dependent optical observation in the austenitic and martensitic state.

Additional features of the role of magnetic domains on the MSM repsonse will be presented.

Funding through the DFG priority program SPP1239 and the National Science Foundation, grant DMR0354740, MW is gratefully acknowledged. We also thank Prof. Kakeshita and Dr. Fukuda for providing the crystal.

MM 23.50 Tue 14:45 Poster B

Molecular dynamics simulation study of crystal growth and melting of pure metals — •Roberto Rozas and Juergen Horbach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, 51147 Köln

The crystallization of Ni is studied by non-equilibrium molecular dynamics simulation. Interactions between atoms are described by a potential of the embedded atom type (EAM). As an initial configuration particles are placed in an elongated simulation box where the crystalline fcc phase in the middle is surrounded by the undercooled liquid phase, separated by two interfaces. The temperature dependence of the interfacial growth is determined by two methods; (i) a global method based on the evolution of the density, (ii) a local method based on a common neighbor analysis and the cone algorithm. The three crystal orientations (100), (110) and (111) are considered. Effects associated with technical aspects of the simulation, such as the influence of thermostat and barostat on crystal growth, are also investigated.

MM 23.51 Tue 14:45 Poster B

USAXS measurements of undercooled charged colloidal model systems — •Ina Klassen[1], Patrick Wette[1], Dirk Holland-Moritz[1], Dieter M. Herlach[1], Thomas Palberg[2], and Stephan V. Roth[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55128 Mainz, Germany — [3]HASYLAB, DESY, 22603 Hamburg, Germany

We analyzed a colloidal system of charged silica particles in aqueous dispersion. The crystallization of charged colloids is driven by strong long- range electrostatic interactions between the particles. The main parameter governing the interaction is the surface charge number of the particles that can be varied in a controlled way by addition of sodium hydroxide.

Our system is characterized by convenient time scales of seconds and particle distances of microns and thus accessible by simple, yet powerful optical techniques. Microscopy and light scattering yield complementary information on equilibrium properties and crystallization kinetics from real and reciprocal space (phase behaviour, solidification mechanisms, growth velocities, nucleation rate densities). With these results we can determine the degree of undercooling of our system. Structural changes of the melt with increased undercooling and the corresponding changes of the solidification can be monitored by Ultra Small Angle X-Ray Scattering (USAXS) performed at Hasylab (Hamburg).

MM 23.52 Tue 14:45 Poster B

Elasticity and solidification kinetics in a eutectic-like two component colloidal system — •Nina J. Lorenz and Thomas Palberg — Institute of Physics, University of Mainz, Germany

Colloidal systems of charged spherical particles in deionized aqueous suspension show a first order phase transition to a crystalline state (bcc or fcc) once the strength and range of the screened Coulomb repulsion are sufficiently large. Recently we also investigated the phase behaviour of binary charged mixtures using static light scattering, to find random composition bcc crystals at charge and size ratios close to one, the onset of compound formation at ratios below 0.7 and a eutectic-like phase behaviour at ratios around 0.55 with strong indications of a gravitation assisted demixing [1]. The kinetics of the latter mixture was monitored via the evolution of the shear elasticity employing torsional resonance spectroscopy. While the pure components and the mixtures far from the eutectic composition solidify via homogeneous nucleation within a few minutes, closer to the eutectic composition the shear modulus takes days to reach its final value in the completely solidified state. We discuss the coupling of crystallization kinetics to the kinetics of demixing, which depend on both the composition and the 'undercooling' which for our systems is approximately linear in particle concentration.

[1] N.Lorenz, J.Liu, T. Palberg: Phase behaviour of binary mixtures of colloidal charged spheres, Colloids Surf. A (in press 2007)

MM 24: SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling III

Time: Wednesday 14:00–15:30 Location: H 1058

Invited Talk MM 24.1 Wed 14:00 H 1058

Nanoscaled domain structures and magnetization processes in thin films — •Volker Neu, Cristina Bran, Felix Fleischhauer, Aarti Singh, Ulrike Wolff, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

Magnetic thin films and multilayers display a fascinating variety of domain structures and magnetization processes due to competing interactions. For single layers one has to consider intra- and intergrain exchange interactions and magnetostatic interactions versus complex anisotropies. In multilayer systems, additional interlayer interactions (e.g. exchange bias, antiferromagnetic or ferromagnetic coupling) broaden the range of possible coupling scenarios and thus the diversity of the magnetic behavior.

For a microscopic understanding of the magnetization processes we perform magnetic force microscopy (MFM), which offers a direct observation of the domain structure on a length scale down to 10 nm, and its evolution in a magnetic field. We present multilayers with perpendicular anisotropy and antiferromagnetic interlayer coupling of the type $[(\mathrm{Co/Pt})_X\mathrm{Co/Ru}]_N$, which possess complex antiferromagnetically and ferromagnetically coupled domain structures, depending on temperature and magnetic history. As an example of a highly anisotropic single layer film with in-plane easy axis orientation, the magnetization process of a nanocrystalline epitaxial $SmCo_5$ film is investigated. Whereas the magnetizing process proceeds on a small length scale of 100 nm, in the demagnetizing process the switching occurs via a fast propagation of few interaction domain walls.

Invited Talk MM 24.2 Wed 14:30 H 1058

Coherent Control of Spin Torque Dynamics — •Hans Werner Schumacher[1], Santiago Serrano-Guisan[1], Karsten Rott[2], Günter Reiss[2], Jürgen Langer[3], and Berthold Ocker[3] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — [2]University of Bielefeld, Universitätsstr. 25, D-33615 Bielefeld — [3]Singulus Nano Deposition Technologies GmbH, Hanauer Landstr. 103, 63796 Kahl am Main

We study time resolved precessional magnetization dynamics induced by spin momentum transfer in nanopillars of CoFeB/MgO/CoFeB magnetic tunnelling junctions (MTJ). Spin transfer torque precession of the CoFeB free layer is excited by ultra short current pulses (0.1 to 5 ns duration) with current densities around 10^6 A/cm2. The time resolved precession of the free layer is studied by measuring the time resolved magneto resistance change of the MTJ using a fast sampling oscilloscope. Our setup allows both to detect the spin torque precession during the current pulse and the magnetization ringing after pulse termination. From the decay of the precession we can derive the effective Gilbert damping parameter of the MTJ free layer. We show that by adapting the duration of the excitation pulse to integer multiples of the period of the spin torque precession the magnetization ringing can be coherently suppressed. Such coherent control of spin torque dynamics is a prerequisite for ultra fast ballistic spin transfer torque magnetization reversal.

Invited Talk MM 24.3 Wed 15:00 H 1058

KeV-He-ion bombardment induced magnetic modifications and patterning of magnetic thin film systems — •Arno Ehresmann — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Str.40, D-34132 Kassel, Germany

The exchange bias effect in antiferromagnet/ ferromagnet magnetic thin film systems results from the exchange interaction at the interface between both materials. Recently a method has been developed to

initialize and tailor the exchange bias in direction and absolute magnitude by bombardment with light ions in a magnetic field [1]. The origin of this effect is a combination of interface and anisotropy modification in the magnetic thin films by the impinging ions. In combining ion bombardment with lithographical techniques a lateral magnetic patterning essentially without change of the surface topography becomes feasible. Besides a brief review of the currently discussed model for the keV-He-ion bombardment induced effects [2], examples for the various possibilities to apply these technique will be given, i.e. among others, tailoring magnitude and direction of the magnetic reference electrode's magnetization in giant magneto and tunnel magneto resistance layer stacks, production of standard samples to magnetically characterize magnetic force microscopy probe tips in in-plane magnetic fields, and positioning of magnetic particles.

Refs.: [1] A. Ehresmann, Recent Res. Devel. Applied Physics 7, 401-21 (2004), [2] A. Ehresmann, D. Junk, D. Engel, A. Paetzold, K. Röll, J. Phys. D. 38, 801-6 (2005)

MM 25: SYM Thin Film Magnetic Materials: Microstructure, Reaction and Magnetic Coupling IV

Time: Wednesday 16:00–17:50 Location: H 1058

Invited Talk MM 25.1 Wed 16:00 H 1058

Magnetic thin film materials tailored by ion irradiation — •Jürgen Fassbender — Forschungszentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 128, 01328 Dresden, Germany

In recent years the tailoring of magnetic properties by means of ion irradiation techniques has become fashionable. Since the magnetic properties of multilayers depend sensitively on the mutual interfaces a modification of these interfaces by ion irradiation leads to a local modification of the magnetic anisotropy, the exchange bias or the interlayer exchange coupling [1,2]. Also structural phase transitions can be induced by ion irradiation. If these are accompanied by magnetic phase transformations ferromagnetic regions can immediately be written with a focused ion beam. In addition to pure radiation effects also doping effects can be exploited to achieve a pure magnetic patterning. Finally ion erosion of semiconductor substrates can be used as periodically modulated substrates which modify the magnetic anisotropies of subsequently deposited magnetic films. Examples of all different approaches will be presented in order to demonstrate the large viability of ion beam technology to tailor magnetic materials.

Refs.: [1] J. Fassbender, D. Ravelosona, Y. Samson, J. Phys. D 37, R179 (2004). [2] J. Fassbender, J. McCord, J. Magn. Magn. Mater. 320, 579 (2008).

MM 25.2 Wed 16:30 H 1058

Magnetic microstructures produced by local ion irradiation induced interfacial mixing — •Thomas Strache[1], Jörg Grenzer[1], Jürgen Fassbender[1], Wolfhard Möller[1], Rainer Kaltofen[2], and Ingolf Mönch[2] — [1]Forschungszentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 128, 01328 Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung IFW Dresden, Institute for Integrative Nanoscience, P. O. Box 270116, 01171 Dresden, Germany

Ion irradiation of $Ni_{80}Fe_{20}/Ta$ multilayers induces an interfacial mixing of these two materials, which subsequently leads to a suppression of the ferromagnetic properties. In order to quantify the structural change grazing incidence x-ray reflectometry has been used. The ion irradiation induced intermixing has been studied by means of TRIDYN simulations. The broadening of the interfaces due to intermixing causes an enrichment of Ta in $Ni_{80}Fe_{20}$ and finally an amorphization of $Ni_{80}Fe_{20}$ above a Ta concentration of 10 to 20 percent [1]. Consequently the ferromagnetic properties are altered or even suppressed completely for high enough ion fluences. It is observed that the critical ion fluence for a complete suppression of the ferromagnetism depends sensitively on the number of interfaces. It is demonstrated that pure magnetic microstructures can be easily fabricated by local ion irradiation without changing the substrate topography.

[1]J. Fassbender *et al.*, Nucl. Instr. and Meth. in Phys. Res. B 248, 343 (2006).

MM 25.3 Wed 16:50 H 1058

Influencing the magnetic properties of NiMn/Co exchange bias system by pulsed laser irradiation — •Senthilnathan Mohanan[1], Ulrich Herr[1], Ralf Diebolder[2], and Raimund Hibst[2] — [1]Insitut für Mikro- und Nanomaterialien, Universität Ulm, 89081 Ulm — [2]Institut für Laseranwendungen in der Medizin und Meßtechnik, Universität Ulm, 89081 Ulm

NiMn with L10 ordered structure is a promising antiferromagnetic material that can be used to achieve exchange bias in giant magnetoresistive spin valve sensors. However, as-deposited NiMn exhibits the paramagnetic fcc phase and has to be annealed at an elevated temperature to obtain the L10 ordered antiferromagnetic fct phase. We present a study on the influence of ns pulsed laser irradiation using a Nd-YAG laser on the structural and magnetic properties of NiMn/Co exchange bias system [1]. X-ray diffraction spectra revealed that upon laser irradiation there is an improvement of the (111) texture of NiMn accompanied by grain growth, but no structural phase transformation. As-prepared and laser irradiated samples were subsequently annealed at different temperatures, and we observed increased exchange bias fields for the laser irradiated samples as compared to those of the as-prepared samples. Since no difference in the degree of ordering was found between as-prepared and laser irradiated samples after annealing, we attribute the observed increase in the exchange bias fields to the modified microstructure.

1. S. Mohanan, R. Diebolder, R. Hibst, and U. Herr, J. Appl. Phys. (accepted)

MM 25.4 Wed 17:10 H 1058

Strain effect on spin reorientation of epitaxial Nd-Fe-B films — •Ah-Ram Kwon[1], Volker Neu[1], Vlakimir Matias[2], Jens Hänisch[2], Ruben Hühne[1], Bernhard Holzapfel[1], Ludwig Schultz[1], and Sebastian Fähler[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden — [2]Los Alamos National Laboratory, Mail Stop T004, Los Alamos NM 8545 USA

Nd-Fe-B is the best permanent magnetic materials known to date. Thin film applications such as magnetic microactuators and motors as well as the study of intrinsic properties require well textured Nd-Fe-B films. Here a new approach to study the influence of strain on the intrinsic magnetic properties, especially spin reorientation transition is demonstrated. Hastelloy, which has high ductility, is used as substrate to reach a strain up to 2% by conventional mechanical elongation. Prior to elongation, MgO(001) had been deposited by ion beam assisted deposition. As a next step Mo and Nd-Fe-B are deposited at 450 °C by pulsed laser deposition. Mo grows epitaxially with a (001) orientation and Nd-Fe-B films onto this buffer possess the desired (00l) out-of-plane orientation. Elongation breaks the symmetry compared to the as-deposited state, resulting in an elliptical shape of the cone opening during spin reorientation. By this novel approaches high strains are obtained which allows to examine highly anisotropic materials where magnetostriction can usually be neglected.

MM 25.5 Wed 17:30 H 1058

Ion damage during FIB-milling of nanostructures into magnetite thin films — •Anjela Koblischka-Veneva[1] and Michael R. Koblischka[2] — [1]Institute of Functional Materials, Saarland University, P. O. Box 151150, D-66041 Saarbrücken, Germany — [2]Institute of Experimental Physics, Saarland University, P. O. Box 151150, D-66041 Saarbrücken, Germany

Nanostructures are prepared into magnetite (Fe3O4) thin films grown on (0 0 1) MgO substrates by means of focused ion beam (FIB) milling. The resulting ion damage is analyzed using the electron backscatter diffraction (EBSD) technique enabling the determination of crystal orientation with a spatial resolution of about 40 nm. Depending on the ion currents and radiation dose applied during the FIB milling, different types of damage are observed. Only at relatively low ion currents, the nanostructures can be created without causing damage to the surrounding magnetite film. This enables the creation of e.g., markers in

order to relocate a given sample section in different experiments like EBSD and magnetic force microscopy (MFM). At high ion currents, an entire ring area around the fabricated nanostructure is affected by the ion beam. The EBSD analysis reveals that new, small grains with a distinct, different orientation pattern are created within the ring area. This could be used to create sample areas with a distinct orientation with respect to the remainder of the magnetite film.

MM 26: Liquid and Amorphous Metals I

Time: Wednesday 14:00–15:15 Location: H 0107

MM 26.1 Wed 14:00 H 0107

Diffusion of Nickel atoms in liquid Silicon — •Anja Ines Pommrich[1], Andreas Meyer[1], Dirk Holland-Moritz[1], and Tobias Unruh[2] — [1]Institut für Materialphysik im Weltraum, DLR, Köln — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRMII), Garching

For the production of Silicon wafers for solar cell applications the knowledge of impurity diffusion of metal atoms in liquid Silicon is necessary to describe the directional solidification process. We measured the Nickel diffusion in liquid Silicon by quasielastic neutron scattering on the TOFTOF-spectrometer of the FRMII in Munich. Electromagnetic levitation was used for container-less processing. This allows diffusion measurements not only in the equilibrium melt but also in the undercooled melt with temperatures up to 280 K below the melting point.

First results show a fast Nickel diffusion as compared to other alloy systems. Furthermore the Nickel self-diffusion coefficients exhibit within error bars no concentration dependence in the range of 5 at% to 20 at% of Nickel and an Arrhenius type temperature dependence.

MM 26.2 Wed 14:15 H 0107

Viskositätsmessungen an flüssigen ternären Cu-Ni-Co Legierungen — •Michael Schick und Ivan Egry — Deutsches Zentrum für Luft- und Raumfahrt, Institut für Materialphysik im Weltraum, 51170 Köln

Für flüssige ternäre Cu-Ni-Co Legierungen wurden mit einem Hochtemperaturviskosimeter [1] die temperaturabhängigen Viskositäten für verschiedene Zusammensetzungen gemessen. Grundlage des Messverfahrens ist die Schwingtiegelmethode [2]. Hierbei wird die in einem Tiegel befindliche Metallschmelze zu einer gedämpften Drehschwingung angeregt. Aus der Dämpfung der Amplitude und der Periodendauer der Schwingung lässt sich mit der Gleichung von Roscoe [2] die Viskosität der Schmelze berechnen. Aus der Temperaturabhängigkeit der Viskositäten können mit Hilfe eines Arrhenius-Ansatzes die Aktivierungsenergien des viskosen Flusses in Abhängigkeit von der Zusammensetzung bestimmt werden. Ein Vergleich der aus den Messungen bestimmten Aktivierungsenergien mit denen, die durch Linearkombination aus den Aktivierungsenergien der reinen Elemente Cu, Ni und Co berechnet wurden, erlaubt Rückschlüsse auf das Mischungsverhalten der Legierungen.

[1] M. Kehr, W. Hoyer, I. Egry: Int. J. Thermophys. 28 (2007) 1017
[2] R. Roscoe: Proc. Phys. Soc. 72 (1958) 576

MM 26.3 Wed 14:30 H 0107

Diffusion of ^{32}P, ^{57}Co and ^{103}Pd in the glass-forming $Pd_{43}Cu_{27}Ni_{10}P_{20}$ alloy and its relation to viscosity — •Alexander Bartsch[1], Klaus Rätzke[1], Andreas Meyer[2], and Franz Faupel[1] — [1]Technische Fakultät, Univ. Kiel, Kaiserstr.2, 24143 Kiel — [2]Institut für Materialphysik im Weltraum, DLR Köln

Since the development of bulk metallic glasses there has been considerable research effort on these alloys. Due to the high stability against crystallisation the undercooled melt between melting temperature and caloric glass transition temperature is now accessible so that recent theories can be tested.

In general, the Stokes-Einstein equation is well accepted in the equilibrium melt of these alloys. In the supercooled melt a decoupling of diffusivity and viscosity around the critical temperature of the mode coupling theory is observed [1]. Now the ^{32}P, ^{57}Co and ^{103}Pd diffusion were measured in a temperature range from 573 K up to 800 K in the $Pd_{43}Cu_{27}Ni_{10}P_{20}$ alloy using the radiotracer technique. We found that P and Co have similar diffusivities and compared them to viscosity data using SE equation [2]. This shows that the mobility of P and Co do not determine the viscosity in the supercooled state. Based on ongoing experiments with ^{103}Pd we now can give an overview on the relation between diffusion and viscosity of all constituents of the alloy.

[1] V. Zöllmer, K. Rätzke, F. Faupel, A. Meyer, Phys. Rev. Lett., 90, 195502-1 (2003).
[2] A. Bartsch, K. Rätzke, F. Faupel, A.Meyer, Appl. Phys. Lett. 89, 121917 (2006)

MM 26.4 Wed 14:45 H 0107

Effect of composition on crystallization behavior and viscosity of Zr-based metallic glasses — •Sergio Scudino, Birgit Bartusch, and Jürgen Eckert — IFW Dresden, Institut für Komplexe Materialien, Postfach 27 01 16, D-01171 Dresden, Germany

The variation of Al and Zr drastically affects the crystallization behavior and the viscosity of the melt-spun Zr-Ti-Nb-Cu-Ni-Al glassy ribbons. The devitrification of the ribbons with high Zr or low Al contents is characterized by the formation of a metastable quasicrystalline phase during the first stage of the crystallization process. With increasing Al or decreasing Zr contents the temperature range of stability of the quasicrystals decreases and their formation is progressively hindered. The temperature of the glass transition and the crystallization temperatures related to the crystallization events shift to higher values with increasing Al or decreasing Zr contents. At the same time, the viscosity of the supercooled liquid and the fragility parameter (D) increase, indicating an improved glass forming ability. A clear correlation between fragility parameter and glass transition has been found. This correlation provides a guide for the estimation of D for this particular system when the glass transition is known.

MM 26.5 Wed 15:00 H 0107

FeNbB bulk metallic glass: the influence of fluxing technique — •Mihai Stoica[1], Santosh Kumar[1,2], Stefan Roth[3], Shanker Ram[2], Jürgen Eckert[1], and Alain Reza Yavari[4] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]Materials Science Centre, Indian Institute of Technology, Kharagpur 721302, India — [3]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — [4]LTPCM-CNRS, Institut National Politechnique de Grenoble, 1130 Rue de la Piscine, BP 75, Saint Martin dHères Campus 38402, France

Recently, a new Fe-based BMG containing only 3 elements and a very high boron ($Fe_{66}Nb_4B_{30}$) content was synthesized. The preparation of this BMG was done by employing the copper mould casting method and using the fluxing technique. This new BMG is ferromagnetic, with a Curie temperature around 550 K and a saturation magnetization of 105 emu/g. Differential scanning calorimetry (DSC) investigations revealed a reduced glass transition temperature of 0.58 and an extension of the supercooled liquid region of about 31 K, values which indicate a relatively good thermal stability. Fluxed and not-fluxed master alloys were used to cast samples. The present work aims to discuss, for both kinds of samples, the kinetics of the phase formation using the Kissinger analysis and Johnson-Mehl-Avrami plots, correlated with the results obtained from X-ray diffraction (XRD) of samples with different metastable structures. Additionally, the magnetic behaviour of different phase(s) will be discussed.

MM 27: Liquid and Amorphous Metals II

Time: Wednesday 15:45–17:00 Location: H 0107

MM 27.1 Wed 15:45 H 0107

Synthesis and mechanical properties of Al-Ni-La alloys prepared by hot extrusion and spark plasma sintering of gas atomized powders — •Kumar Babu Surreddi[1], Hoang Viet Nguyen[2], Mira Sakaliyska[1], Sergio Scudino[1], Mihai Stoica[1], Markus Wollgarten[3], Ji-Soon Kim[2], and Jürgen Eckert[1] — [1]IFW Dresden, Institut für Komplexe Materialien, Postfach 270116, D-01171 Dresden, Germany — [2]Research Center for Machine Parts and Materials Processing, University of Ulsan, Namgu Mugeo 2-Dong, San 29, Ulsan 680-749, Republic of Korea — [3]Hahn-Meitner-Institut Berlin, Glienicker Straße 100, D-14109 Berlin, Germany

Bulk nanocrystalline Al87Ni8La5 specimens were prepared by in-situ devitrification and consolidation of gas atomized glassy powders. Consolidation was carried out at different temperatures by hot extrusion as well as by spark plasma sintering (SPS). Both techniques lead to highly dense bulk specimens with a microstructure consisting of an fcc-Al phase together with several intermetallic compounds. The powders consolidated by SPS display the highest compression strength, which depends on the consolidation temperature and ranges between 900 and 1000 MPa, together with plastic strains not exceeding 10 %. The extruded samples are characterized by a maximum strength of about 800 MPa but generally show larger plastic strains that can reach values of about 20 %. These results indicate that the mechanical properties of the samples can be tuned within a wide range of strength and ductility as a function of the consolidation technique and parameters used.

MM 27.2 Wed 16:00 H 0107

Phase formation and mechanical properties of $Cu_{50}Zr_{50-x}Ti_x$ ($2.5 \leq x \leq 7.5$) glass matrix composites — •Simon Pauly, Jayanta Das, and Jürgen Eckert — IFW Dresden

The microstructure and elastic/plastic properties of $Cu_{50}Zr_{50-x}Ti_x$ ($2.5 \leq x \leq 7.5$) glass matrix composites have been investigated. The presence of austenitic (Pm-3m)/martensitic phases (P21/m and Cm) with different length scales embedded in a glassy matrix enhances the plastic deformability significantly. These composites show high yield strength (up to 1753 MPa) and large plastic strain (over 15 %). The high strength scales with the volume fraction of glassy matrix and the ability of these alloys to undergo an austenite-martensite transformation is believed to be beneficial for increasing the intrinsic ductility of the BMGs.

Furthermore, the evolution of phases upon annealing ribbons of the aforementioned compositions has been studied and the crystallization kinetics has been determined using Kissinger and Johnson-Mehl-Avrami analysis. The fragility parameter of different compositions has been correlated with their plastic behavior as well as the Poisson's ratio.

MM 27.3 Wed 16:15 H 0107

Study of complex elastic moduli of metallic glasses during relaxation processes and in confined geometry — •Dennis Bedorf[1], Thomas Koeppe[1], Konrad Samwer[1], and Ranko Richert[2] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Chemistry and Biochemistry, Arizona State University, Tempe AZ 85287- 1604, USA

Measuring the complex elastic constants in a metallic glass enables us to study relaxation processes especially during the first heating run of a glass. The first increase of storage modulus far below the alpha process can be linked to a beta process. The different rate dependence of both can be used to estimate the merging temperature [1]. Dynamical heterogeneities are known to have spatial dimension of several nm. To get experimental data of loss spectra in confined geometry we measure thin films of PdCuSi on a double-paddle-oscillator (DPO). Change of resonance frequency and Quality factor are used to determine the complex shear modulus of the film. Preparation and characterizations were performed in situ under UHV conditions. Precise measurements of early relaxations above RT were also performed by using thin cantilevers of a metallic glass. All results are discussed in the model of a potential energy landscape as described in [2]. This work was supported financially by DFG, SFB 602 and Leibniz Programm.

[1] J. Hachenberg et al., to be published

[2] J. S. Harmon, M. D. Demetriou, W. L. Johnson and K. Samwer, Phys. Rev. Lett. 99, 135502 (2007)

MM 27.4 Wed 16:30 H 0107

Dynamics of Shear Transformation Zones in Metallic Glasses — •Max Neudecker and S. G. Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Dynamical heterogeneities in metallic glasses are investigated for the model glass, $Cu_{50}Ti_{50}$, with the help of classical molecular dynamics computer simulations. By rapid quenching from melt at various cooling rates (comprising 5 orders of magnitude), differently relaxed amorphous cells are prepared. During a subsequent shearing, macroscopic properties (particularly the stress-strain curve) are linked to microscopic dynamics. We find the global shearing is composed of highly localized shear events, termed shear transformation zones (STZs), which occur spatially and temporally inhomogeneously. A detailed analysis focuses on the origins and implications of STZ formation.

Financial support by SFB 602 (project B3) is gratefully acknowledged.

MM 27.5 Wed 16:45 H 0107

Strain- and Temperature-induced Glass-to-Crystal Transformations in Al-Ni-La Glass — •Jens Vierke[1], Gerhard Schumacher[1], Ingwer A. Denks[1], Nelia Wanderka[1], Markus Wollgarten[1], John Banhart[1], Ivo Zizak[2], Vitaly P. Pilyugin[3], Martin Balog[4], Juray Nagy[4], and František Simančik[4] — [1]Hahn-Meitner-Institute Berlin, Germany — [2]BESSY Berlin, Germany — [3]Ural Branch of the Russian Academy of Sciences, Yekaterinburg, Russia — [4]Slovak Academy of Sciences, Bratislava, Slovakia

Helium-atomized amorphous Al85Ni10La5 powders were consolidated using uni-axial pressing, equal channel angular pressing (ECAP) and high pressure torsion (HPT) at temperatures ranging from room temperature to 400°C. The samples were investigated by scanning electron microscopy (SEM), in-situ angle-dispersive (AD) and ex-situ energy-dispersive (ED) X-ray diffractometry (XRD) and differential scanning calorimetry (DSC). As-atomized powders show a glass transition and a subsequent simultaneous crystallization of fcc-Al and intermetallic phases upon continuous and isothermal heating. Samples consolidated below the crystallization temperature show only fcc-Al nanocrystals and a residual amorphous phase. They exhibit no glass transition upon continuous heating. The amount of fcc-Al nanocrystals increases with strain and processing temperature as revealed by ED XRD measurements along the disc radius of a HPT-sample and by AD XRD along the pressing direction of ECAP-samples stopped halfway in the ECAP-die. The results indicate that the primary precipitation of fcc-Al is strain-induced and possibly athermal.

MM 28: Intermetallic Phases I

Time: Wednesday 17:30–18:15 Location: H 0107

MM 28.1 Wed 17:30 H 0107

Investigation of lead free soldering reaction between solid Ni and liquid Sn — •Jens Görlich and Guido Schmitz — Institut für Materialphysik, Wilhelm-Klemm-Str.10, D-48149 Münster, Germany

After the ban of lead it is important to understand the reaction mechanisms of new lead free solder systems. We investigated the interreaction between solid Ni and liquid Sn. Reaction times were from 10 seconds to 14 days at 250°. By scanning electron microscopy we obtained the particle size distributions and determined grain growth of the Ni_3Sn_4 phase with time. With focused ion beam preparation, we could study the properties of the intermetallic connection layer

at the interface Ni/Sn by transmission electron microscopy (TEM) in detail. At short times, the growth rate agrees with the flux driven ripening theory for soldering [1] [2], but for longer times, the time exponent deviates significantly. TEM analysis reveals that the general assumption of constant interface area is not fulfilled at any time. We will compare the experimental data with existing soldering models and present an approach for the growth kinetics of Ni_3Sn_4 in the Ni/Sn system.(supported by DFG)

[1] K.N. Tu et. al., Physical Review B 66, 115403 (2002)
[2] G. Gosh, J. Appl. Phys. Volume 88, Nr. 11 p.6887

MM 28.2 Wed 17:45 H 0107

Fabrication of CoTiSb and NbNiSb Half-Heusler phases for thermoelectric applications — NOTE: This talk has been withdrawn — •Wilfried Wunderlich, Yoshikaji Aoki, Kousuke Nakatsuka, Hideto Ueno, and Yuichiro Motoyama — Tokai University, Fac. Eng, Materials Science Dept., Hiratsuka-shi, Kanagawa, Japan

Important applications of Half-Heusler phases are as thermoelectric materials. For the cases of CoTiSb, TiNiSn and others, ab-initio simulation using VASP-software could confirm the phase stability against phases with concurrent crystal structures like TiNiSn, ZrCoAl, ZrBeSi, FeSiV and Full Heusler. However, the thermo dynamical driving force for formation as calculated from the difference in lattice energies is less than 0.1eV/atom. Hence, the fabrication of Half heusler phases is difficult and requires three steps, surface activation of the raw material by ball milling, arc-melting of pressed pellets and finally long-term annealing treatment. For the CoTiSb system, diffusion couple experiments clarified the complicated diffusion mechanism, which can lead in worst cases to Kirkendahl voids and constitutional vacancies. On doped CoTiSb specimens, Seebeck coefficients up to 0.1 mV/K, on NiNbSb 0.3 mV/K were measured.

MM 28.3 Wed 18:00 H 0107

Influence of microstructure on magnetostriction properties of FePd thin films — NOTE: This talk has been withdrawn — •Wilfried Wunderlich, Keisuke Takahashi, Daiji Kubo, Yoshihito Matsumura, and Yoshitake Nishi — Tokai University, Fac. Eng, Materials Science Dept., Hiratsuka-shi, Kanagawa, Japan

FePd-alloys as thin films are potential actuators materials due to their magnetostriction. Experiments and simulations of TEM and XRD diffraction patterns showed, that the L1_0-ordering has no influence on the lattice parameter ratio c/a=1.37. The degree of long-range order is higher for the sputtering temperature of 573K than of 423K, but the magnetostriction is higher for thin films produced at 423K. The model for explanation is contrary to the usual behavior, where ordering increases the magnetic susceptibility; for acchieving a large magnetostriction an initial degree of disorder is more favorable.

MM 29: Mechanical Properties I

Time: Wednesday 14:00–15:15 Location: H 0111

MM 29.1 Wed 14:00 H 0111

Molecular Dynamics Simulations of Grain Boundary Plasticity — •Yvonne Ritter, Alexander Stukowski, and Karsten Albe — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

Dislocation nucleation at grain boundaries (GB) and as well as grain boundary sliding are relevant mechanisms governing the deformation behavior of nanocrystalline metals. By means of molecular dynamics simulations we examine well defined bicrystal geometries under different loads. The simulations are performed for copper and aluminum in order to investigate the influence of various stacking fault (SF) energies. For a Σ 7 (111) twist boundary GB sliding occurs by a collective movement of all atoms in the boundary plane, but no dislocation activity can be detected. A Σ 33 (225) tilt boundary with a dissociated structure dos not deform by GB sliding but reacts by the growth of pre-existing intrinsic stacking fault facets when exposed to a shear deformation. Under tensile deformation partial dislocations nucleate from both GBs. The nucleation mechanism is thermally activated in both cases. In the case of the Σ 7 GB the dislocations are statistically emitted from tetrahedral nucleation sites. The partial dislocations, that are emitted from the Σ 33 GB, emerge at well defined positions determined by the GB structure.

MM 29.2 Wed 14:15 H 0111

Micropillars compression test — •Nousha Kheradmand, Afrooz Barnoush, and Horst Vehoff — Saarland University Bldg. D22 P.O. Box 151150, Postcode D-66041, Saarbruecken, Germany

In order to investigate the size effect compression test of single crystal micropillars was performed. Micropillars with different crystallographic orientations were fabricated by focused ion beam and the compression test was performed in a nanoindenter utilizing a flat punch tip. As a new approach in order to observe the micropillars in their intermediate deformation conditions, the compression test was performed stepwise. Between each step the micropillars were imaged in a scanning electron microscope. The engineering stress-strain curves of the micropillars show a clear size effect on mechanical properties of the samples. The small samples show a linear elastic-perfectly plastic deformation followed by incremental strain bursts, while the larger samples show a continuously flow curve. This difference could be described by a so called source truncation strengthening model which occurs in samples with small diameter. According to this model a Frank-Read source line during the growth reaches the free surface before it is able to be multiplicated. This leaves two single-arm dislocations which are pinned from one end inside the sample and from the other end on the free surface. These dislocations introduce to the samples new yield stresses.

MM 29.3 Wed 14:30 H 0111

Determination of intrinsic stresses in thin films by nanoindentation — •Olena Chukhrai[1], Andre Clausner[1], Norbert Schwarzer[2], and Frank Richter[1] — [1]Chemnitz University of Technology, Institute of Physics, Chemnitz, Germany — [2]SIO - Saxonian Institute of Surface Mechanics, Eilenburg, Germany

Intrinsic stresses often occur in thin films as a result of the complex formation of the thin film structure. Therefore, simultaneous determination of intrinsic stress and yield strength are necessary. It was shown [1], that intrinsic stresses can be derived from nanoindentation data by combination of "pure normal"and mixed (normal and tangential) loading, in particular, when the concept of the "effectively shaped indenter"is used. A device for creation of biaxial stress in the samples which can be used together with our nanoindentation setup (UNAT, Asmec GmbH) was constructed, tested and utilized for the investigation of a highly elastic Ni/Ti alloy. We found that for the NiTinol hardness changed by more than 70% when the stress was varied between 0 and 0.9 GPa. Using our theoretical concept [1], the intentionally introduced biaxial stress could be taken into account and the yield strength could be determined. The next step was to apply for the samples with known biaxial stress a combination of "pure normal"and mixed loading with pointed indenter and to determine the intrinsic stress and the yield stress using our theory. The feasibility of the concept of simultaneous determination of intrinsic stresses and yield strength by nanoindentation was shown and it can now be used.

[1] Schwarzer N.: http://archiv.tu-chemnitz.de/pub/2006/0018/index.html

MM 29.4 Wed 14:45 H 0111

In situ tensile testing of nanocrystalline Pd and Pd-Ag alloys — •Kejing Yang[1], Julia Ivanisenko[2], Jürgen Markmann[3], and Hans-Jörg Fecht[1,2] — [1]Institute of Micro and Nanomaterials, University of Ulm, D-89081 Ulm, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — [3]Universität des Saarlandes, FR7.3 Technische Physik, Saarbrücken, Germany

Arising from a low strain hardening ability, the limited uniform elongation of nanocrystalline materials (NC) hinders the further improvement of their mechanical properties. In this study we suggest a way to enhance strain hardening by purposefully alloying Pd to reduce its stacking fault energy (SFE). Nanocrystalline Pd and Pd-Ag alloys were prepared by high-pressure torsion. Tensile testing was carried out in situ in a high-resolution SEM to investigate the mesoscopic deforma-

tion process at a strain rate of 10-3 s-1. The NC alloys demonstrated very high values of strength and ductility. The true stress-true strain curves exhibit a larger strain hardening effect and larger uniform deformation in Pd-Ag alloys than in pure Pd. We relate this enhanced behavior to a decreased SFE in the alloys: the lower the SFE, the more difficult is the cross slip and climb of split dislocations, which leads to greater dislocation storage and, ultimately, to increased strain hardening. The dimpled structure of fracture surfaces in the alloys will also be discussed in relationship to these findings.

MM 29.5 Wed 15:00 H 0111

New approach to design the strain hardening ability in nanostructured materials. (exchanged with MM 30.1) — •Lilia Kurmanaeva[1], Yulia Ivanisenko[1], Jürgen Markmann[2], Jörg Weissmüller[1,2], Ruslan Z. Valiev[3], and Hans-Jörg Fecht[4] — [1]Institute für Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany — [2]Universität des Saarlandes, Saarbrücken, Germany — [3]Institute of Phisycs of Advanced Materials, Ufa, Russia — [4]Institute of Micro and Nanomaterials, University of Ulm, Ulm, Germany

The recent past has seen an increasing interest in studies of mechanical properties of nanostructured materials(NSM), since new methods of continuous processing of bulk NSM using severe plastic deformation were developed. NSM demonstrate superior hardness and strength, but often a limited ductility due to poor strain hardening(SH) ability. In present paper we suggest a simple method to increase the SH ability of NSM by decreasing the stacking fault energy(SFE). The microstructure and mechanical properties of nanocrystalline Pd and Pd-x%Ag(x=5,10,20,40) alloys were investigated. Additions of Ag strongly decrease the SFE of Pd. The initially coarse grained samples were processed by high pressure torsion, which resulted in formation of homogeneous ultrafine-grained structure. The increase of Ag contents led to the decrease of the resulted grain size. Consequently, the samples with larger Ag contents demonstrated the higher values of strength properties. The uniform elongation had also increased, and tensile curves exhibited larger SH. Thus we have obtained a combination of high strength and good ductility in nanostructured Pd-Ag alloy.

MM 30: Mechanical Properties II

Time: Wednesday 15:45–17:00 Location: H 0111

MM 30.1 Wed 15:45 H 0111

Tensile tests of magnetron sputtered nanocrystalline palladium (exchanged with MM 29.5) — •Anna Castrup[1,2], Sebastian Gottschalk[1], Horst Hahn[1,2], Rudolf Baumbusch[3], Patric Gruber[3], and Oliver Kraft[3] — [1]Institute of Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany — [2]Institute for Materials Science, Thin Films Division, Darmstadt University of Technology, Petersenstr. 23, D-64287 Darmstadt, Germany — [3]IZBS, University of Karlsruhe, Kaiserstr. 12, 76131 Karlsruhe, Germany

Nanocrystalline Pd films of 1 μm thickness were prepared by rf magnetron sputtering on Kapton substrates. The films were sputtered by use of nanoscale multilayer technology with individual deposition layer thicknesses ranging between 1 and 20 nm at various sputter conditions.

The resulting grain size and texture were characterized using TEM and conventional XRD measurements. Tensile tests were performed ex-situ as well as in-situ in a synchrotron diffractometer. Peak form analysis reveals intrinsic and extrinsic stacking fault density and twin density, which depend on the applied strain rate. Considered deformation mechanisms are: grain boundary sliding, grain rotation and the formation of stacking faults. It is investigated whether the formation of these defects is reversible after relaxation.

MM 30.2 Wed 16:00 H 0111

Fe-based composite materials with improved mechanical properties — •Katarzyna Werniewicz[1,2], Uta Kühn[1], Norbert Mattern[1], Jürgen Eckert[1], Ludwig Schultz[1], and Tadeusz Kulik[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Warsaw University of Technology, Faculty of Materials Science and Engineering, Warsaw, Poland

Following a previous study by the authors two new compositions $(Fe_{89.0}Cr_{5.5}Mo_{5.5})_{91}C_9$ and $(Fe_{89.0}Cr_{5.5}Mo_{5.5})_{83}C_{17}$ have been developed with the aim of improving the ductility of $Fe_{65.5}Cr_4Mo_4Ga_4P_{12}C_5B_{5.5}$ bulk metallic glass (BMG). In contrast to the alloys in that study, the recently prepared Fe-based materials are Ga-free. It was expected that the variations in the composition will lead to the changes in the phase formation and, hence, in the mechanical response of the investigated alloys. It was recognized that in-situ formed Fe-based composites show superior plasticity ($\epsilon_{pl} \approx 37\%$) for the alloy with lower C content and ($\epsilon_{pl} \approx 4\%$) for the alloy with higher C content compared to monolithic glass ($\epsilon_{pl} \approx 0.2\%$). Furthermore, on the basis of present as well as previous investigations it has been shown that the Ga addition is beneficial for the plasticity of these Fe-based alloys. It was observed that the $(Fe_{89.0}Cr_{5.5}Mo_{5.5})_{83}C_{17}$ alloy exhibits a significantly smaller fracture strain ($\epsilon_f \approx 5\%$) compared to its Ga-containing counterpart ($\epsilon_f \approx 16\%$). Therefore, it can be concluded that appropriate alloying additions are crucial in enhancing the mechanical properties of the complex Fe-based materials developed here.

MM 30.3 Wed 16:15 H 0111

Mechanical Characterisation of a human tooth with a structured filling material — •Ferenc Molnar[1], Frank Richter[1], and Norbert Schwarzer[2] — [1]Chemnitz University of Technology, Solid State Physics, 09107 Chemnitz, Germany — [2]Saxonian Institute of Surface Mechanics, Lieschow 26, 18569 Ummanz, Germany

New materials for dental use must have mechanical properties comparable to those of the surrounding biological material. To investigate a structured filling material consisting of hard nanometer-sized grains in a tough matrix with high local resolution we have applied the method of nanoindentation. Therefore a cross-section of the tooth has been prepared and depth sensing indentation measurements were performed. Using the UNAT device (Universal Nanomechanical Tester, Asmec GmbH) with a Berkovich indenter an array of totally about 3200 measuring points with a spacing of 75 microns were created covering the essential parts of the tooth including filling, dentine and dental enamel regions. Young's modulus and hardness have been determined for each point of this array to obtain laterally resolved data of these mechanical properties. In addition, we have evaluated the yield strength of the filling material applying the effective indenter approach of Schwarzer [J. Phys. D: Appl. Phys., 37 (2004) 2761-2772]. The filling shows quite homogeneous behaviour to the external load but at smaller scales the microstructure gains more influence. Values of hardness and Young's modulus for particular measuring points being by a factor of two or three bigger than the average could be correlated by optical microscopy to single extraordinary large grains in the matrix.

MM 30.4 Wed 16:30 H 0111

Simulation der ersten Phasen der Materialermüdung durch ein granulares Modell — •Judith Fingerhuth[1], Matz Haaks[1], Gunter Schütz[2] und Karl Maier[1] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

Basierend auf der Idee des zellulären Automaten werden die ersten Phasen der Ermüdung eines Metalls vor der Initiierung von Mikrorissen mit einem mesoskopischen Modell simuliert. Der Kristall wird dabei als regelmäßige Anordnung von Kristallkörnern betrachtet, deren komplexe, individuelle Eigenschaften durch die skalaren Parameter Korngröße, Orientierung und Schädigung (mittlere Versetzungsdichte pro Korn) repräsentiert werden. Die Schädigung eines Korns wird aus der plastischen Verformung, der pro Verformungszyklus dissipierten Energie und Schädigung der Nachbarkörner berechnet. In einer eindimensionalen Implementierung wurde das Verhalten von Nickel im einachsigen Zug-Druck-Versuch teilweise wiedergegeben. Es werden nun die Ergebnisse einer realistischeren 2D-Implementierung vorgestellt.

MM 30.5 Wed 16:45 H 0111

Vorhersage des Ermüdungsbruchs an vordeformiertem Karb-

onstahl — •Patrick Eich[1], Matz Haaks[1], Karl Maier[1] und Ralf Sindelar[2] — [1]Helmholtz- Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, 53115 Bonn — [2]FH Hannover, Ricklinger Stadtweg 120, 30459 Hannover

Die Ermüdung und das Versagen verschiedenster Bauteile unter Wechselbelastung spielen in Industrie und Forschung eine wichtige Rolle. Da die Lebensdauer unter zyklischer Belastung begrenzt ist, wäre eine präzise Schadensvorhersage von großer Bedeutung.
Die physikalische Ursache für die Ermüdung von metallischen Legierungen ist die Akkumulation von Gitterfehlern, wie Versetzungen, und durch Versetzungsbewegung erzeugte Defekte.
An der Bonner Positronen Mikrosonde lässt sich die von der Wechselbelastung verursachte Zunahme der Defektdichte mit der Methode der Positronen-Annihilations-Spektroskopie ortsaufgelöst messen. Dadurch kann der Ermüdungszustand bei höheren Lastzyklenzahlen aus der Defektdichte im Anfangsstadium der Ermüdung abgeschätzt werden [1].
Für Proben des Karbonstahls C45E, die sich zu Beginn der Belastung im ausgeheilten Materialzustand befinden, lässt sich aus den Frühstadien der Ermüdung die Restlebensdauer mit zu Wöhlermethoden vergleichbarer Sicherheit abschätzen. Um diese Vorhersagemethode unter realistischen Bedingungen zu testen, wurde die gleiche Versuchsreihe an vordeformierten Proben durchgeführt.

[1] M.Haaks, K. Maier in V. Jentsch et al. “extreme events”

MM 31: Mechanical Properties III

Time: Wednesday 17:30–18:30 Location: H 0111

MM 31.1 Wed 17:30 H 0111

Inhomogeneous flow characteristics of bulk metallic glasses — •Alban Dubach, Florian Dalla Torre, and Jörg Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Wolfgang-Pauli-Str. 10, 8093 Zurich, Switzerland

In contrast to crystalline metals, which exhibit dislocation mediated deformation, bulk metallic glasses (BMGs) bear a high resistance to plastic flow at low temperatures (T) but viscous like properties close to their glass transition temperature. Both mechanical responses underlie a single mechanism: nucleation and propagation of shear transformation zones (STZs). As opposed to high T deformation at low T is temporarily and spatially restricted within narrow shear bands and therefore difficult to assess experimentally and less well understood.

In this study the inhomogeneous flow kinetics of Zr-based BMGs are investigated at sub-ambient T by strain rate change tests and the temporal and spatial characteristics of shearing are compared with the appearance of shear bands and fracture surfaces. Using the time durations of individual shear events an ”apparent viscosity” at the moment of shearing can be estimated. Our results show that serrated flow, typically observed at room temperature, disappears below a critical T or above a critical strain rate, in accordance with a change of the strain rate sensitivity. A constitutive model for inhomogeneous flow in BMGs is presented which describes the deformation behaviour according to a thermally activated (cooperative) motion of STZs, including a time varying state variable representing the local state of relaxation in the shear band.

MM 31.2 Wed 17:45 H 0111

Predicting deformation localisation in cellular materials — •John Dunlop[1], Richard Weinkamer[1], Yves Bréchet[2], and Peter Fratzl[1] — [1]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Research Campus Golm, 14424, Potsdam, Germany — [2]Groupe Physique du Métal, SIMAP INPG, Domaine Universitaire de Grenoble, 38402 Saint Martin d’Hères, France

Cellular and porous solids fail under compressive loading through the nucleation and propagation of localised deformation bands throughout the material. In ordered cellular solids such as trabecular bone, wood, as well as in honeycombs and three dimensional periodic lattices localisation or crush bands form in which the localisation plane has a specific orientation with respect to the lattice architecture and the applied load. This has a strong similarity to martensitic phase transformations in atomic crystals which can be described by the propagation of elastic instabilities along particular weak crystallographic directions. The instabilities of atomic crystals were first studied by Born, and there is now a well developed theory available to describe and analyse such structures. In this contribution the lattice dynamics theory is applied to beam lattices of different architectures in order to predict the direction of deformation localisation beam lattices of different architectures in two and three dimensions.

MM 31.3 Wed 18:00 H 0111

Monte Carlo Simulation of Segregation Including Elastic Relaxations — •Rolf Anders and Ferdinand Haider — Universität Augsburg, Institut für Physik

We developed a real space technique which includes local atomic relaxation after each MC step, allowing thus to study processes with strong elastic contributions. The MC step consists of a vacancy jump, exchange of nearest neighbours or atom type change. The activation energy is computed using phenomenological interaction potentials (Lennard-Jones or EAM). After an accepted MC step the atomic coordinates in the vicinity of the modification are relaxed in order to minimise the total energy.

Using this method, segregation to lattice defects was simulated in NiAl and FeNi alloys. In the case of grain boundaries, the temperature dependence of the interfacial excess concentration was studied. It was found to be in good agreement with the Langmuir-McLean theory.

For an edge dislocation, the pinning force due to segregation was calculated. This was accomplished by shifting the concentration profile along the Burgers vector and subsequent relaxation of the lattice.

MM 31.4 Wed 18:15 H 0111

Mechanical properties of Pb-free solder-joints — •Jan Keller[1], Guido Schmitz[1], and Ulrich Wilke[2] — [1]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany — [2]Infineon Technologies AG, Max-Planck-Str. 5, 59581 Warstein, Germany

After the prohibition of lead the main focus in packaging technology is to improve the performance of electronic devices. A critical issue is the mechanically stability. From the new relevant lead free solders regarding melting point and wettability, one has to figure out the composition with the best mechanically properties. In this work, we investigate the mechanical strength of $Sn_xAg_yCu_z$-solder between Cu-substrates with different contents of Ag and Cu in Sn. After soldering reactions under reducing atmosphere the solder joints are sheared and stress-strain curves are recorded. Mechanically loaded and unloaded specimens are observed by optical and scanning electron microscopy to determine the fracture structure and the reasons for the failure. The maximum strength, fracture toughness and elongation are related to the observed microstructure.(supported by Infineon Technologies AG)

MM 32: HV Fähler

Time: Thursday 9:30–10:00 Location: H 1058

Invited Talk MM 32.1 Thu 9:30 H 1058

Magnetic Shape Memory Alloy Films: What is different to bulk materials? — •Sebastian Fähler — IFW Dresden, Institute for Metallic Materials, P. O. Box 270116, 01171 Dresden, Germany

Bulk single crystals made of magnetic shape memory alloys reach strains up to 10% when applying a moderate magnetic field below 1 T. When these materials have easily moveable twin boundaries, reorientation of martensitic variants can occur. Variants having the easy magnetization axis along the field direction can grow preferentially. Due to the different axis length of the martensitic unit cell, a macro-

scopic change of length can be obtained. After summarizing the phenomenology of this effect for bulk single crystals, the different behavior observed in thin, epitaxial Ni-Mn-Ga and Fe-Pd films is analyzed. It is shown that the substrate influences several properties. First the film orientation can be controlled by epitaxy. Additionally a biaxial stress with respect to the substrate induces the martensitic transition. The boundary condition towards a rigid substrate reduces the number of observed variants. Though no macroscopic strain is expected in constrained films, it is shown that the additional free parameter of an orthorhombic structure allows a magnetically induced microstructure reorientation within a film even though its overall dimensions are constrained by the substrate. Additionally first experiments on free standing films are presented, showing the influence of a rigid substrate on phase formation and variant orientation.

This work is supported by DFG through SPP 1239 "www.MagneticShape.de"

MM 33: SYM Hydrogen in Materials: New Developments I

Time: Thursday 10:15–11:25 Location: H 1058

Invited Talk MM 33.1 Thu 10:15 H 1058

Hydrogen Physisorption in MOFs — •Barbara Panella[1,2] and Michael Hirscher[2] — [1]Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, Hönggerberg, Zürich, Switzerland — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Metal-organic frameworks (MOFs) are due to their extremely high porosity and defined structure very attractive materials for hydrogen storage at cryogenic temperatures (77 K). The storage capacity of molecular hydrogen in MOFs is higher than for any other porous material and further improvements are expected if the framework structure of novel MOFs will be optimized. This optimization can involve different routes like increasing the specific surface area, tuning the size of the pores and introducing metal centers which might strongly polarize the molecule. This presentation will give an overview on the most important results obtained in the last years on hydrogen storage in MOFs focusing on the correlation between structure and hydrogen adsorption properties. Additionally, a comparison between MOFs and other classes of porous materials for hydrogen physisorption will be presented. Finally several experimental techniques will be shown which allow to investigate the interaction between hydrogen and metal-organic frameworks.

MM 33.2 Thu 10:45 H 1058

Isosteric heat of adsorption for hydrogen in microporous materials — •Barbara Schmitz[1,2] and Michael Hirscher[1] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Universität Bonn, Germany

The adsorption of hydrogen in activated carbon and metal organic frameworks is measured with an automated Sieverts apparatus. The pressure dependent hydrogen uptake is investigated at several temperatures above 77K and pressures up to 20bar. The total uptake is correlated to the specific surface area. From the adsorption isotherms the isosteric heat of adsorption is evaluated within a wide range of surface coverage between 0.2 and 0.8. The results are related to the structure of the different materials.

Acknowledgment: Partial funding by the European Commission DG Research (contract SES6-2006-518271/ NESSHY) is gratefully acknowledged by the authors.

MM 33.3 Thu 11:05 H 1058

Hydrogen storage in nanoporous materials — •Sergei Yurchenko[1], Lyuben Zhechkov[1], Thomas Heine[1], Aliezer Martinez[1], Gotthard Seifert[1], and Serguei Patchkovskii[2] — [1]Institut für Physikalische Chemie und Elektrochemie, TU Dresden, D-01069 Dresden, Germany — [2]Steacie Institute for Molecular Sciences, NRC Canada, 100 Sussex Drive, Ottawa, Ontario, K1A 0R6 Canada

In this study we investigate the effect of the structural characteristics of the nanoporous environment on the hydrogen abundance in the material. For this purpose we evaluate the hydrogen adsorption in well-defined hypothetical systems as well as in realistic environment, which have been studied in experiment before. We calculate storage capacity of the adsorbed hydrogen gas at different conditions, varying the gas temperature and pressure.

For our simulations we employ the quantized liquid density functional theory (QLDFT), developed recently as an extension of the density functional theory of liquids to quantized liquids at finite temperatures. We introduce a reference fluid of non-interacting featureless hydrogen molecules obeying Boltzmann statistics in connection with the rigorous Kohn-Sham formulation. Following the liquid DFT this functional is extracted from thermodynamical experimental data for uniform hydrogen fluids. Thus the method allows us to take into account directly the interaction between the hydrogen molecules, which usually is a large source of errors for systems with highly inhomogeneous guest density.

MM 34: SYM Hydrogen in Materials: New Developments II

Time: Thursday 11:40–12:50 Location: H 1058

Invited Talk MM 34.1 Thu 11:40 H 1058

The Interaction of Hydrogen with Metal Surfaces: Molecular Precursors, Chemisorbed Atoms and Subsurface States — •Klaus Christmann — Institut für Chemie und Biochemie der FU Berlin, 14195 Berlin

In this contribution, the scenario of hydrogen interaction with (single-crystalline) metal surfaces will be surveyed including physisorbed and chemisorbed molecular hydrogen, dissociative (atomic) hydrogen adsorption, and subsurface H state population, whereby both energetic and kinetic phenomena will be considered. Special attention is devoted to H-induced structural changes of the surface region of the exposed crystal (relaxation and reconstruction), on subsurface state population and especially on molecularly chemisorbed hydrogen. Relatively strongly bound adsorbed hydrogen molecules may play an important role as a precursor during H uptake and storage processes, and recent results obtained for H and H2 interacting with the (210) surfaces of the fcc metals Ni, Pd and Rh will be presented.

MM 34.2 Thu 12:10 H 1058

Thermodyamic aspects of the hydrogen absorption in nanometallic clusters — •Mohammed Suleiman, Reiner Kirchheim, and Astrid Pundt — Institute of Material Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

Metallic nano-sized clusters (2.0-6.0 nm) have been shown to have distinct differences in their hydrogen uptake characteristics when compared to bulk Pd. These differences are not only due to the different physical properties of the small-size system but they could be affected by the stabiliser and, also, by the cluster structure. In this work the thermodynamic absorption behaviour of hydrogen in nm-sized metallic clusters with different size and different structure will be presented. The phase transition in these samples was monitored by in situ X-ray diffraction and in situ EXAFS measurements during hydrogen loading. The thermodynamic behaviour of hydrogen absorption will be presented using P-c Isotherm, P-d Isotherms and P-R Isotherm. It will be shown that the phase boundaries and the hydrogen uptake ability in these samples depends strongly on the lattice structure which is affected by the type of metallic clusters and the stabilizer used in samples.

MM 34.3 Thu 12:30 H 1058

MC-MD simulations of pressure-concentration isotherms for Hydrogen in bulk Palladium and clusters — •Diana Marcano

and Helmar Teichler — Institut fuer Materialphysik, Universitaet Goettingen

For nanoscale Pd clusters loaded with H experimental pressure - concentration isotherms resemble those for bulk material, with the main difference of a finite slope instead of the two-phase regime and a narrowing of this region compared to bulk. Regarding this, we here present results from MC-MD studies using for the chemical potential a new calculation scheme, which means an extension of Widom's particle insertion method. The simulations rely on the Tomanek model with improved H-Pd coupling for properly taking care of lattice deformations and modified H-H interaction including first and second neighbour interactions. For bulk material, the asymmetric two-phase regime is obtained, extending up to 62 % H. The results for a 923 Pd atoms cuboctahedral cluster reflect the variation of site energies in the cluster where the shift to lower H concentrations is related to the interplay between first and second neighbour H-H interactions.

MM 35: Phase Transitions I

Time: Thursday 10:15–11:15 Location: H 0107

MM 35.1 Thu 10:15 H 0107

Magnetostrain in polycrystalline 5M Ni50Mn29Ga21 — •Uwe Gaitzsch, Martin Pötschke, Claudia Hürrich, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Magnetic shape memory alloys have been investigated due to the coupling of magnetic and mechanical properties. By moving twin boundaries in the martensitic state, magnetic-field-induced strain (MFIS) of at maximum 10 % can be achieved. So far, MFIS has only been shown in single crystals. To provide a suitable polycrystalline mircostructure, directional solidification was employed to get a coarse-grained, textured sample. These samples were heat treated for chemical homogenization and stress relaxation. In Ni50Mn29Ga21 samples with 5M crystal structure could be prepared. Structural characterization and texture investigations have been performed using X-ray diffraction techniques. Cubic samples were cut erosively from the ingots to allow for mechanical training via cyclic compression along different axes. One of the sample axes was along the direction of solidification. The training leads to a reduction of the twinning stress by over an order of magnitude as compared to an untrained sample. At the same time the mechanical strain could be increased to the crystallographic limit of 1- c/a. After training in a modified Instron testing machine their magnetic-field-induced strain was measured. By appropriate training up to 1 % of MFIS could be achieved in polycrystalline samples.

Financial support by the DFG within SPP 1239 is gratefully acknowledged.

MM 35.2 Thu 10:30 H 0107

Controlling the microstructure in NiMnGa alloys — •Martin Pötschke, Franziska Thoss, Uwe Gaitzsch, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, Helmholzstr. 20, 01069 Dresden

NiMnGa alloys have gained large research interest because of their possible application as magnetic shape memory materials. This effect is caused by the motion of twin boundaries in a magnetic field. So far, this effect has only been demonstrated in single crystals. However, the preparation of single crystals is a time consuming and cost intensive process and compositional changes along the crystal axis as well as segregations may occur. This is why for technical applications there is a great interest in polycrystals. To extend this effect to polycrystals, directional solidification was applied in order to prepare coarse grained, textured samples. The martensitic transformation temperature which strongly depends on the composition was monitored by DSC, and it is shown that the chemical homogeneity along the sample axis is improved in likewise treated samples. The preferred solidification-induced growth direction was determined by EBSD. Additional annealing steps which are necessary to further improve the chemical homogeneity, coarsening of grains, and stress relaxation effect the texture. Investigations on the texture development during annealing are discussed.

Financial support by the DFG within SPP 1239.

MM 35.3 Thu 10:45 H 0107

Ferromagnetic shape memory alloy Mn_2NiGa: — •Guodong Liu and Claudia Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz

The structure, martensitic transformation and magnetic properties of $Mn_{25+x}Ni_{50-x}Ga_{25}$ ($x = 0 \cdots 25$) alloys were detailedly investigated. It was found that these alloys favour the Hg_2CuTi-type structure instead of the conventional Cu_2MnAl-type structure. All the samples go through a martensitic transformation on cooling. The transformation temperatures (TM) of the samples with $x > 12.5$ are different from the conventional electron concentration rule. The stoichiometric Mn_2NiGa exhibits a TM of around room temperature and a lattice distortion as large as 21.3% upon the martensitic transformation and has a quite high Curie temperature of 588 K. Excellent two-way shape memory behavior and magnetic-field-controlled effects were observed in Mn_2NiGa single crystals. The electronic structures of Mn_2NiGa were calculated by the first-principle method. The results show that Mn_2NiGa alloy is ferrimagnetic due to antiparallel but uncompensated magnetic moments of Mn atoms at different sublattices in austenite. Furthermore, is shown for off-stoichiometric samples that additional Mn atoms substituting Ni atoms in Ni_2MnGa have the same magnetic behavior as Mn in the Mn_2NiGa phase, which explains the dependence of the magnetization on the Mn composition. (Goudong Liu acknowledges the support by the Institute of Physics, Chinese Academy of Sciences in Beijing and the fellowship by the Humboldt Stiftung.)

MM 35.4 Thu 11:00 H 0107

Dynamic observation of ac field induced twin boundary motion in bulk NiMnGa — •Ryan Yiu Wai Lai, Jeffrey McCord, Rudolf Schaefer, and Ludwig Schultz — Leibniz-Institute for Solid State and Materials Research, P.O.Box 270116, Dresden D-01171, Germany

A study of actuating performance in bulk NiMnGa magnetic shape memory single crystals at various frequencies is presented. A dynamic actuation experimental setup with the ability to apply mechanical stress and alternating magnetic field perpendicularly is developed in cooperation with time-resolved microscopy. Reversible twin boundary motion activated in the frequency range up to 600Hz is directly observed. The maximum field induced strain increases with actuation frequency. Strain hysteresis curves show a pronounced dependency on actuation frequency. The mechanism of the frequency response will be discussed in detail. Funding through the DFG priority program SPP1239 is gratefully acknowledged.

MM 36: Phase Transitions II

Time: Thursday 11:45–13:00 Location: H 0107

MM 36.1 Thu 11:45 H 0107

First Principles Investigation of Twin Boundary Motion in Magnetic Shape Memory Heusler Alloys — •Markus Ernst Gruner and Peter Entel — Fachbereich Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

In the martensitic phase of the magnetic shape memory (MSM) Heusler alloy Ni_2MnGa, strains of up to 10 % can be induced by external magnetic fields, making the material a technologically relevant candidate for magneto-mechanical actuators. The MSM effect in near stoichiometric Ni_2MnGa is connected with a modulated pseudotetragonal martensitic phase with $c/a < 1$. It is attributed to a high mobility of the twin-boundaries in connection with a large magneto-crystalline

anisotropy allowing the reorientation of martensitic twins with the help of a magnetic field thereby changing the shape of the crystal. So far, the origin of the high mobility of twin-boundaries in this phase is unresolved and empirical potentials permitting the simulation on the relevant length and time scales do not exist. We therefore attempt to close this gap by large scale ab initio calculations in the framework of density functional theory allowing the investigation of simplified models of martensitic twin boundaries for the different martensitic structures of Ni_2MnGa with the help of contemporary supercomputers. First results indicate that for the low-temperature, non-modulated martensitic $L1_0$ structure with $c/a > 1$, the energy needed for shifting a twin boundary is too large to be overcome by magneto-crystalline anisotropy.

[1] M. E. Gruner, P. Entel, I. Opahle, M. Richter, J. Mater. Sci. (accepted for publication)

MM 36.2 Thu 12:00 H 0107

Strain measurements in ferromagnetic martensitic Heuslers and magnetization easy axis — •Seda Aksoy, Mehmet Acet, and Eberhard F. Wassermann — Experimentalphysik, Universität Duisburg-Essen, Duisburg, Germany

The temperature-dependence of strain under constant magnetic-fields is studied in Ni-Mn-X (X: Ga, In, Sn, Sb) and Ni-Mn-In-X (X: Ga, Sn, Sb) polycrystalline ferromagnetic Heusler alloys which undergo a martensitic transformation close to room-temperature. The applied magnetic-field influences the nucleation of martensite so that decreasing the temperature under a magnetic field leads to large length changes between the austenite and martensite states. The length-change within the martensitic state varies with the magnitude of the cooling-field. This is related to the variant-orientation during martensite nucleation. These strain-data provide information on the easy axis of magnetization.

MM 36.3 Thu 12:15 H 0107

Phase transformations of Ni_2MnGa shape memory alloy from first principles. — •Matthe' Uijttewaal, Tilmann Hickel, and Joerg Neugebauer — MPI für Eisenforschung, Düsseldorf, Germany

Ni_2MnGa is a typical example of a Heusler alloy that undergoes a martensitic transformation. The high-temperature austenite has a cubic $L2_1$ structure, whereas below 200 K the structure is orthorhombically distorted. The transformation is completely reversible despite lattice deformations of up to 10% and large strains connected to this change. Ni_2MnGa is attractive for application in actuators and sensors because magnetism can control its phases. Central to the shape memory properties is a soft phonon mode in the austenite, leading to modulated (pre-) martensitic phases. Despite ample research, the physics of this soft mode is not well understood. We, therefore, systematically studied the soft mode in the various phases (austenite, pre-martensite and modulated martensites) and their transitions using ab initio DFT (GGA, PAW). First, phonon spectra were computed in the quasiharmonic approximation. The eigenvectors of the unstable phonon modes were used next to set up the corresponding modulated harmonics in supercell calculations and to identify the stable shuffling structures. Based on the derived double-well potentials we successfully explained the mechanism of the transitions and determined the corresponding temperatures. We conclude that for the pre-martensitic transition the dynamics of the phonons are important. The resulting temperature dependence of the phonon frequencies compares favorably to available neutron scattering experiments for this material.

MM 36.4 Thu 12:30 H 0107

Beyond the standard analysis of magnetic shape memory alloys-Comparison of Ni-Fe-Ga and Ni-Mn-Ga single crystals — •Oleg Heczko[1], Alexander Vasiliev[2], Yuriy Chumlyakov[3], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P. O. Box 27 01 16, 01171 Dresden, Germany — [2]Moscow State University, Moscow, 119991, Russia — [3]Tomsk State University, Tomsk, 634050, Russia

Some ferromagnetic Heusler alloys exhibiting martensitic transformations are known to change their shape by an external magnetic field (MSM effect). Here we analysed in depth and compared the magnetic properties of Ni54Fe19Ga27 and Ni50Mn29Ga21 single crystals; at low temperature using Bloch spin wave theory, at high temperature in the vicinity of the ferromagnetic transition using the equation of state and Arrot analysis. Temperature dependence of reciprocal paramagnetic susceptibility indicates a ferrimagnetic ordering in Ni-Fe-Ga compound. Magnetic anisotropy is determined from the magnetization curves measured in different temperatures. The transformation to martensitic phase is accompanied by the increase of the spontaneous magnetization and large increase of magnetocrystalline anisotropy in both compounds. The consequences of observed differences of magnetic properties for existence of the MSM effect are discussed.

MM 36.5 Thu 12:45 H 0107

The study on the structure, magnetism and shape memory effect of the ferromagnetic shape memory alloy CoNiGa. — •Xuefang Dai and Claudia Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz

The structure, magnetic properties and shape memory effect of CoNiGa alloys were investigated in the bulk, as-spun and single crystal samples. It was found by experiments that the ternary CoNiGa alloys have good shape memory effect, and the shape memory strain can be easily controlled by temperature, magnetic field and stress. For optimizing the mechanical properties, the iron was doped in the CoNiGa alloys. Excellent superelasticity was obtained in the quaternary CoNiFeGa single crystal samples. The superelastic strain of 6.7% can be induced by compressed stress and 11% can be obtained in tension test. In addition, the perfect superelasticities also showed up in bending and torsion tests. Special CoNiFeGa crystals with regular defects have also been grown in a deep super-cooling condition. These defects result in a large energy barrier which leads to a very sharp martensitic transformation within a temperature window of only 2 K. On the other hand, we also prepared Si-doped CoNiGa alloys, which exhibit larger magnetic-field-induced strain than the ternary CoNiGa alloys. This improvement in magnetic-field-induced strain can be attributed to the increase of the magnetic anisotropy induced by the Si-dopant.

Xuefang Dai acknowledges the support by the Institute of Physics, Chinese Academy of Sciences, Beijing 100080.

MM 37: Intermetallic Phases II

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

MM 37.1 Thu 10:15 H 0111

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

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

MM 37.2 Thu 10:30 H 0111

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

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

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

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

MM 37.3 Thu 10:45 H 0111

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

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

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

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

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

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

MM 37.4 Thu 11:00 H 0111

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

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

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

This work is supported by the "Studienstiftung des deutschen Volkes" which is gratefully acknowledged.

MM 38: Nanostructured Materials V

Time: Thursday 11:45–13:00 Location: H 0111

MM 38.1 Thu 11:45 H 0111

Single crystalline metal nanowires with high aspect ratio — •Achim Walter Hassel and Srdjan Milenkovic — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Directional solidification of eutectics with an asymmetric composition is a route to metallic nanowires. This coupled growth yields a single crystalline matrix with embedded single crystalline nanowires, all being aligned parallel to each other. Differential electrochemical processing allows a partial, local or entire release of the wires with an aspect ratio of over 1000. Various metals can be used such as the refractory metals Re, Mo and W or the noble metals Au and Cu. Both, diameter and length can be controlled by the processing parameters in a wide range. Prototypes for further investigations and applications will be shown.

MM 38.2 Thu 12:00 H 0111

The influence of ion irradiation on bimetallic nanoparticles — •Darius Pohl[1], Elias Mohn[1], Jürgen Fassbender[2], Karsten Albe[3], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Forschungszentrum Rossendorf, D-01314 Dresden, Germany — [3]TU Darmstadt, D-64287, Germany

FePt nanoparticles with mean diameters of about 5 nm and a narrow particle size distribution are prepared through inert gas condensation. Since as-deposited particles usually exhibit the metastable disordered and soft magnetic A1 phase or even other structural motifs such as icosahedral or decahedral multiply twinned structures, additional annealing steps are required to transform these particles into the $L1_0$ phase.

In order to gain more insight into the phase stability of the various crystal structures observed in FePt nanoparticles we have investigated, how ion irradiation influences these structures. Comparable studies were conducted on particles of CuAu, the phase diagram of which is very alike that of FePt. In the present study, gas-phase prepared single crystalline and multiply twinned FePt and CuAu nanoparticles are irradiated with ions of different noble gases and different energy. It is shown that the He^+ ion irradiation promotes the de-twinning of the bimetallic nanoparticles and the formation of single crystalline A1 phase particles. A comparison of the experiments on CuAu nanoparticles with the results of molecular dynamic simulations will be presented. The effect of the energy difference between the different morphologies for both the ordered and disordered structures is discussed.

MM 38.3 Thu 12:15 H 0111

Sintering of Metallic Nanoparticles — •Ralf Meyer and Peter Entel — Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

With the growing interest in the production of nanoparticles with well defined physical properties for novel technological applications, the sintering of nanoparticles has become an increasingly important subject. In this work, the sintering of metallic nanoparticles is studied at temperatures of 800 and 1000 K over periods of up to 200 ns with the help of molecular-dynamics simulations. Simulations of the sintering of two Ni nanoparticles with diameters of approximately 4 nm show that a small-angle grain boundary with a corresponding (partial) dislocation grid is formed shortly after the particles make contact. The grain boundary remains stable over a period of several nanoseconds, until the dislocations disappear from the system. The disappearance of the disocations leads to a simultaneous rotation of the grains so that a single-crystalline particle is formed. In addition to the simulations of the sintering of two particles, results will be shown of the simulation of the sintering of 300 particles containing several million atoms into a single 40 nm sized particle.

MM 38.4 Thu 12:30 H 0111

Reactive diffusion under elastic stress in nanospheres — •Constantin Buzau Ene[1], Guido Schmitz[2], Carsten Nowak[1], Talaat Al-Kassab[1], and Reiner Kirchheim[1] — [1]Universität Göttingen, Institut für Materialphysik, Friedrich-Hund Platz 1, D-37077 Göttingen — [2]Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str.10, D-48149 Münster

A remarkably clear experiment has been designed in order to investigate the influence of stress on reactive diffusion in spherical symmetry. Thin film Al/Cu/Al and Cu/Al/Cu triple layers with approximately 10 nm single layer thickness are deposited on curved substrates of 25 nm radius and investigated by atom probe tomography. The experiments demonstrate that the reaction rate depends significantly on the deposition sequence of the metals. The thickness of the product formed at the interfaces at which Cu is deposited on top of Al is approximately 1.5 to 2 times thicker than that of the opposite stacking sequence. This observation may be explained naturally by Laplace tension of the curved interfaces. By quantitative analysis, the level of induced stress can be determined from the modified growth rates.

MM 38.5 Thu 12:45 H 0111

Twinning during low-temperature deformation of nanocrystalline pulsed-electrodeposited nickel — •Klemens Reuther, Lutz Hollang, and Werner Skrotzki — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden

Pure 'nanocrystalline' nickel was produced by pulsed electro-deposition without additives for grain refinement. The average grain size of the material is d_{EBSD} = 150 nm and d_{XRD} = 30 nm if determined by electron backscatter diffraction (EBSD) and by X-ray diffraction (XRD), respectively. Tensile tests between 4 K and 320 K reveal that the material is ductile in the whole temperature range. Generally, the stress-strain curves are parabolic and the stress reaches its maximum after about two percent plastic strain, with the ultimate stress strongly increasing with decreasing temperature. However, there exists a critical temperature T_T = 9 K below which the deformation mode suddenly changes towards twinning if the stress level reaches 2400 MPa. The twinning events are characterized by substantial stress drops accompanied by loud acoustic emissions. The microstructural changes connected with twinning will be discussed on the basis of results obtained by scanning and transmission electron microscopy.

MM 39: SYM Hydrogen in Materials: New Developments III

Time: Thursday 14:00–16:00 Location: H 1058

Invited Talk MM 39.1 Thu 14:00 H 1058

Hydrogen Chemisorption to Clusters — •Gerd Gantefoer — Department of Physics, University of Konstanz, Germany

The properties of nanoclusters consisting of up to 100 atoms are different from the ones of the corresponding bulk materials. Their geometric and electronic structures change with each additional atom. As a consequence chemical properties also vary dramatically with size. The interaction of such nanoparticles with hydrogen exhibits a broad variety of new and unexpected effects. E.g., single hydrogen atoms behave like gold atoms if attached to a small Au cluster. The interaction of small Al clusters with atomic hydrogen results in the formation of a new, previously unknown family of Aluminum hydrides. These examples demonstrate, that chemistry of nanoclusters is different and provides a new approach to the problem of hydrogen storage.

Invited Talk MM 39.2 Thu 14:30 H 1058

Hydrogen Storage in Light Weight Metal Hydrides: Mg-based Reactive Hydride Composites — •M. Dornheim, U. Bösenberg, C. Pistidda, G. Barkhordarian, J. Bellosta v. Colbe, and R. Bormann — GKSS-Research Centre Geesthacht, Institute of Materials Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Compared to conventional room temperature hydrides light weight metal hydrides have much higher gravimetric hydrogen storage densities. However, kinetic and/or thermodynamic restrictions limit the potential use of such high capacity hydrides. There is still a large number of hydrides with high storage capacities which have to be considered as irreversible or at least require high pressures and/or very high temperatures for reversible hydrogenation / dehydrogenation as well as very long absorption and desorption times. Prominent examples are borohydrides like $LiBH_4$. Another crucial parameter is the reaction enthalpy. Most of the past attempts to alter and tailor the hydrogen reaction enthalpy of light weight metal hydrides like Mg either failed or led to dramatically reduced gravimetric hydrogen storage capacities. An exciting and promising novel approach is the concept of the Reactive Hydride Composites (RHC). RHC consisting of MgH_2 and borohydrides show significantly reduced total reaction enthalpies as well as improved ab- and desorption kinetics compared to the pure borohydrides while a high hydrogen storage capacity is maintained [1]. In this talk, an overview on the sorption behaviour of the doped nanocrystalline RHCs $2LiBH_4$+MgH_2, $2NaBH_4$+MgH_2 and $Ca(BH_4)_2$+MgH_2 will be given.
[1] Scripta Materialia 56 (2007) 841-846.

MM 39.3 Thu 15:00 H 1058

Direct synthesis of $LiBH_4$ monitored by in-situ neutron diffraction — •Arndt Remhof[1], Oliver Friedrichs[1], Florian Buchter[1], Andreas Züttel[1], and Dirk Wallacher[2] — [1]EMPA, Swiss Federal Laboratories for Materials Resaerch, Dübendorf, Switzerland — [2]Hahn Meitner Institut, Berlin Neutron Scattering Facility, Berlin, Germany

Due to its large hydrogen content, $LiBH_4$ is a promising candidate for a hydrogen storage material. Recently, we discovered a way to synthesize LiBH4 directly from the respective elements, by exposing Li and B to hydrogen gas at high temperatures 700°C and at high pressures (150 bar) [1]. The synthesis can be facilitated by using intermetallic Li-B compounds as starting material. We have shown by in-situ neutron powder diffraction that starting from an intermetallic Li-B compound $LiBD_4$ can be synthesized at 180bar at a temperature of 350°C, which is about 350°C lower than the temperature required for the direct synthesis [1,2]. The experiment was carried out at the powder diffraction instrument E6 of the Hahn Meitner Institut. Support by A. Hoser and N. Stüsser is gratefully acknowledged. Financial support from the 6^{th} Framework Program of the European Commission (NESSHY Contract No.: 518271) and the Swiss Federal Office of Energy is acknowledged.
[1] O. Friedrichs et al., Acta Materialia, in press
[2] D. Goerrig, Deutsches Patent; Auslegungsschrift (1960)

MM 39.4 Thu 15:20 H 1058

Refinement of the phonon analysis in the complex hydride systems $LiBH_4$ and $LiBD_4$ — •Ana Maria Racu[1], Joachim Schoenes[1], Zbigniev Lodziana[2], Andreas Borgschulte[2], and Andreas Züttel[2] — [1]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Germany — [2]EMPA Materials Sciences and Technology, Div. Hydrogen and Energy, Dübendorf, Switzerland

In the present study we have performed low temperature micro Raman measurements on small $LiBH_4$ and $LiBD_4$ crystals. At the lowest temperature, the spectra compare very well with the calculated phonons for the orthorombic structure. The spectra are dominated by three separated bands: the external modes, the internal bending and the internal stretching vibrations. Internal refers to vibrations within the BH_4^- tetrahedra while external modes imply motions of Li^+ and BH_4^-. The temperature dependence of the observed phonons corroborates the strong anharmonicity of the system. Due to the anharmonicity, Fermi resonances occur between the first order stretching modes and the second order bending modes of $LiBH_4$. Moreover, the linewidths have an Arrhenius-like component, with an activation energy of 40 meV. This value corresponds to the energy of the librational mode determined by inelastic neutron scattering [1] and is strongly related to the reorientation motions of the BH_4^- tetrahedra.
[1] J. Tomkinson, T. C. Waddington, J. Chem. Soc. Faraday Trans 2 **72**, 528 (1976).

MM 39.5 Thu 15:40 H 1058

Hydrogen release of $Mg(BH_4)_2$ under helium and hydrogen backpressure — •Wiebke Lohstroh, Nobuko Hanada, Christoph Frommen, and Maximilian Fichtner — Institut für Nanotechnologie, Forschungszentrum Karlsruhe GmbH, Postfach 3640, 76021 Karlsruhe

$Mg(BH_4)_2$ is one of the potential materials to be used in solid state hydrogen storage systems due to its high capacity of 14.9 wt% H_2 and a favourable reaction enthalpy. However, experimentally, hydrogen is only released at temperatures above 300 °C. Depending on the surrounding gas atmosphere (helium or hydrogen) and the applied backpressure several decomposition steps are observed. We will present

thermal analysis and structural investigations at various stages of the decomposition and the hydrogen release mechanism will be discussed.

MM 40: SYM Hydrogen in Materials: New Developments IV

Time: Thursday 16:30–18:00 Location: H 1058

Invited Talk MM 40.1 Thu 16:30 H 1058

Complex Metal Hydrides — •Michael Felderhoff — Max-Plack-Institut für Kohlenforschung, Kaiser Wilhelm Platz 1, 45470 Mülheim / Ruhr

One important feature for a commercial success of PEM fuel cell for mobile applications is the improvement of the hydrogen storage system. Since the physical storage methods are limited, solid state hydrogen storage are in the focus of research activities. The classical metal hydrides have storage capacities not higher than 2 wt.%. Compared to these materials the storage capacities of the complex metal hydrides are much higher. Sodium aluminium hydride (NaAlH4) is one of the most interesting material, because it is fully reversible, the thermodynamic properties and the storage capacities are close to the technical requirements for on-board hydrogen storage. The recent work for optimization of the complex metal hydrides and to understand the molecular processes during the de- and rehydrogenation reactions will be summarized.

MM 40.2 Thu 17:00 H 1058

XRD, XPS and Raman analysis of metal and complex hydrides — •Isabel Llamas Jansa[1], Carine Rongeat[1], Steffen Oswald[2], Angelika Teresiak[2], Martin Kalbác[3], and Oliver Gutfleisch[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270016, D-01171 Dresden, Germany — [2]IFW Dresden, Institute for Complex Materials, P.O. Box 270016, D-01171 Dresden, Germany — [3]IFW Dresden, Institute for Solid State Research, P.O. Box 270016, D-01171 Dresden, Germany

X-ray diffraction (XRD), photoelectron spectroscopy (XPS), and Raman spectroscopy, preferentially as in-situ techniques, are valuable tools for the characterisation of the chemical state and structure of doped metal- and complex-hydrides and their intermediate products upon absorption and desorption. Examples for ex- and in-situ characterisation of the evolution with temperature and pressure of doped-$NaAlH_4$ [1] and reactive hydride composites [2] (e.g. $LiBH_4 + MgCl_2$) are discussed. XPS surface analyses indicated the complete decomposition of the catalyst in the case of $TiCl_3$ doped $NaAlH_4$ samples, whereas samples doped with $ScCl_3$ and $CeCl_3$ still showed traces of the chloride phases. Raman results demonstrated the formation of the $Mg(BH_4)_2$ phase after high-pressure ball milling (HP-BM) of a $LiBH_4$ + $MgCl_2$ mixture for 12 h. Finally, in-situ XRD was used to monitor the transition from tetrahydride ($NaAlH_4$) into the hexahydride (Na_3AlH_6) phase during desorption of sodium alanate.

[1] C. Rongeat, I. Llamas-Jansa, and O. Gutfleisch, in preparation (2007)
[2] U. Boesenberg et al., Acta Materialia 55, 3951 (2007)

MM 40.3 Thu 17:20 H 1058

Seeing Hydrogen — •Andreas Borgschulte — EMPA Materials Science and Technology, Hydrogen & Energy, Überlandstrasse 129, CH-8600 Switzerland

The fact that hydrogen absorption in metals leads to large optical changes is the basis of a new combinatorial method called hydrogenography. We show that hydrogenography provides a high-throughput method to measure quantitatively the key thermodynamic properties (equilibrium properties like heat of absorption and kinetics) of hydride formation. The optical setup involves a good accessibility of the sample, which enables us the measurement of the impact of electric fields on the hydrogen absorption process. We demonstrate that an electric current and the thereby induced heat and electromigration of H^- ions can start and control the absorption of hydrogen in Mg thin films. We describe how the optical technique on thin films can be transferred to measure hydrogen dynamics in bulk materials by means of Raman spectroscopy.

MM 40.4 Thu 17:40 H 1058

Opto-mechanical high-throughput characterization of composition spread thin films for the development of new hydrogen storage materials — •Alfred Ludwig[1,2], Jialin Cao[2], Alan Savan[2], Michael Ehmann[2], and Hans-Werner Becker[3] — [1]Institut für Werkstoffe, Ruhr-Universität Bochum — [2]Combinatorial Materials Science, caesar, Bonn — [3]Institut für Physik mit Ionenstrahlen, DTL Labor, Ruhr-Universität Bochum

An opto-mechanical high-throughput characterization method was used for the investigation of hydrogen storage materials within the system Mg-B-Ti-Pd. The materials were deposited by magnetron sputtering in form of thin film composition spreads on micromachined Si cantilever arrays. The thin films were characterized by EDX and XRD prior and after hydrogen loading. In a special pressure vessel, the mechanical stress-changes of the coated cantilevers as a function of hydrogen pressure (0.1 to 5.1 MPa) and temperature (20 to 450°C) was measured in parallel using the optical technique. These stress-changes are related to the hydrogen uptake/release of the different materials. The most promising thin films which showed hydrogen storage were further analyzed by RBS and NRA. The latter was used to determine the hydrogen content of the thin films and its depth distribution.

MM 41: Poster SYM Hydrogen in Materials: New Developments

Time: Thursday 18:00–20:00 Location: Poster B

MM 41.1 Thu 18:00 Poster B

Beyond the featureless particle approximation: An extension of quantum-liquid density-functional theory to account for rotational effects. — •Sergei Yurchenko[1], Serguei Patchkovskii[2], Thomas Heine[1], and Gotthard Seifert[1] — [1]Institut für Physikalische Chemie und Elektrochemie, TU Dresden, D-01069 Dresden, Germany — [2]Steacie Institute for Molecular Sciences, NRC Canada, 100 Sussex Drive, Ottawa, Ontario, K1A 0R6 Canada

In a different contribution we present QLDFT (Quantum Liquid Density Functional Theory), a Kohn-Sham based extension to DFT for liquids, to describe the adsorption properties of molecules in host structures under consideration of quantum effects. In QLDFT the individual molecules are treated as featureless particles, and rotational contributions to the free energy are neglected. However in the vicinity of strong charges the featureless particle approximation breaks down and rotational contributions become important even at ambient conditions.

We present an extension of QLDFT to account for rotational effects. Then, we apply this new method to examine the effect of electric field-induced interactions on hydrogen adsorption. These interactions initiated by the atomic charges are stronger than dispersive interactions and can facilitate the H_2/host binding, which can potentially lead to the increase of the hydrogen adsorption. We present results of simulations of the hydrogen adsorption for a number of model and real structures. We analyze the rotational and spatial probability distributions of the adsorbed hydrogen both with slow and fast varying atomic charge fluctuations.

MM 41.2 Thu 18:00 Poster B

Hydrogen Adsorption in Metal-Organic Frameworks — •Irena Senkovska and Stefan Kaskel — Department of Inorganic Chemistry, Technical University Dresden, Germany

Metal-Organic Frameworks (MOFs) have recently received considerable attention because of their high specific micropore volume and the ability to store gas molecules exceeding the storage capacity of traditional adsorbents. A variety of differences in the MOFs structures makes it difficult to analyze the influence of different factors on

hydrogen uptake capabilities in MOFs. We have investigated the influence of the minor structural changes of the MOFs on their hydrogen storage capacity. The influence of the incorporated metal was shown for following isostructural compounds: $Cu_3(BTC)_2$ (BTC=1,3,5-benzenetricarboxylate) and $Mo_3(BTC)_2$; $Zn_2(BDC)_2DABCO$ and $Co_2(BDC)_2DABCO$ (BDC=1,4-benzenedicarboxylate, DABCO=1,4-diazabicyclo[2.2.2]octane). Our research interest is directed also towards the discovery of new MOFs, as well as adjusting the pore dimensions of MOFs, using different building blocks, solvent and solvent mixtures, in order to improve gas uptake and adsorption properties. Magnesium-based MOFs were found with the same network topology, very small pore size and selective adsorption behaviour. They show a guest-induced reversible structure transformation due to the flexibility of the Mg3-cluster and the organic linkers. This effect could be used for fitting the pore sizes and for the increase of gas sorption capability in Mg contained MOFs after all. The hydrogen adsorption was also studied in several Al-based IRMOFs.

MM 41.3 Thu 18:00 Poster B

H_2 Adsorption in Metal-Organic Frameworks — •Agnieszka Kuc[1], Thomas Heine[1], Gotthard Seifert[1], and Helio Duarte[2] — [1]Physikalische Chemie TU, Dresden, Germany — [2]UFMG, Belo Horizonte, Brazil

We report the results of calculations on molecular hydrogen binding in so called IRMOF-1 (Isoreticular Metal-Organic Framework). MOFs are a new class of porous and stable materials that can act as hydrogen storage media. Density Functional Theory (DFT) was employed for the calculations of geometry of a connector and a linker (building blocks). Complete periodic systems and electronic structure of MOFs were calculated within Density Functional based Tight-Binding (DFTB) method. Second order Møller-Plesset (MP2) perturbation theory was used to calculate the interaction energies between H_2 and model building blocks.

Two different model structures were chosen to mimic the environment of extended IRMOF-1 crystal. Systematic study of the influence of the basis set size on the results was performed. The results were corrected by employing the basis set superposition error (BSSE) to describe more precisely weak interactions. The mixed basis sets were used, depending on the interaction regions. The dipole moments and the electrostatic potential were estimated, as well.

MM 41.4 Thu 18:00 Poster B

Hydrogen on planar and curved graphitic surfaces — •Helmut Hermann, Melanie Hentsche, Andrei Touzik, and Olga Khvostikova — Leibniz-Institute for Solid State and Materials Research IFW Dresden, PF 270116, D-01171 Dresden, Germany

For planar graphene, recent theoretical work has predicted a maximum amount of about 4.5wt% hydrogen storage capacity [1]. Thermodynamic estimates have shown that the storage capacities do not exceed 1wt% at 100K and rapidly decrease at higher temperatures [2]. Experimental investigations of the hydrogen storage capacity of nanostructured graphitic material in the temperature range of 30K to 300K point to the assumption that the storage capacity is considerably enhanced at low temperatures by the presence of small open micropores as compared to planar graphene [3]. Therefore, we are looking for graphitic materials with particularly high fraction of micropores. Expandable graphite seems to be a promising starting material for this purpose.

[1] T. Heine, L. Zhechov, G. Seifert, Phys. Chem. Chem. Phys. 6 (2004) 980.
[2] A. Touzik, H. Hermann, Chem. Phys. Lett. 416 (2005) 137.
[3] M. Hentsche, H. Hermann, D. Lindackers, G. Seifert, Int. J. Hydrogen En. 32 (2007) 1530.

MM 41.5 Thu 18:00 Poster B

Hydrogen loading of nano crystalline niobium thin-films. — •Kai Nörthemann and Astrid Pundt — Institut für Materialphysik, Universität Göttingen

This contribution presents the phase transition in hydrogen loaded nano crystalline thin films.

As model the system of niobium with hydrogen was measured during gas phase loading. The phase transition is monitored in situ with the surface sensitive scanning tunneling microscopy (STM). The α and hydride phase can be distinguish due to the expansion of the hydride phase. We will show the arrangement of the hydride phase in the surrounding α phase. Due to the continuous taken STM images we also show the time dependency of the phase transition.

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

MM 41.6 Thu 18:00 Poster B

Optical and magnetic characterisation of rare earth hydride films — •Helge Schröter, Dirk Menzel, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelssohnstraße 3, 38106 Braunschweig

It is well known that rare earth metals like yttrium or europium show a metal insulator transition, if they are exposed to a hydrogen atmosphere. Yttrium changes from a reflective metal to a very weakly transparent metal (YH_2) and finally to a transparent insulator (YH_3). Europium also undergoes a metal to insulator transition however, in addition a transition from antiferromagnetism to ferromagnetism has been reported to occur in powder samples [1]. Due to the reactivity of the pure rare earth metals it is difficult to grow stable films. We have grown in-situ hydrogenated films of yttrium and europium by pulsed laser deposition in a hydrogen atmosphere. By variation of the hydrogen pressure thereby, we succeeded to grow layers with different hydrogen concentrations. The EuH_x films have been covered in-situ with a gold layer to protect against oxidation and deterioration. After removal from the vacuum chamber the optical and magnetic properties of the films have been determined by spectroscopic ellipsometry and SQUID magnetometry, respectively. The former measurements demonstrate the formation of the optical gap, while the latter indicate an increasing moment with increasing hydrogen content. For the highest hydrogen concentrations a semiconductor with a gap of 1.9 eV and a ferromagnetic transition at 17 K is obtained.

[1] P. Wachter et al. J. Magn. Magn. Mat. 31-34 (1983) 255.

MM 41.7 Thu 18:00 Poster B

Mechanical stress impact on thin films thermodynamic properties - investigated by H-loading — •Stefan Wagner and Astrid Pundt — Institut für Materialphysik der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Thermodynamic properties of thin films deviate strongly from those of bulk. The deviations are reported to originate from microstructure and from mechanical stress, while the contribution of both is unknown in particular. Focussing on the mechanical stress contribution and by using Pd-H and PdFe-H as model systems, it is shown that mechanical stress strongly changes phase transition pressures. For the Pd-H films the measured loading pressures shift up to 140 mbar in contrast to 18 mbar for bulk. These shifts relate to the film bonding to the substrate and can be affected by film detachment.

MM 41.8 Thu 18:00 Poster B

Optimization of the magnetic properties of Co/Pd multilayers by applying a large persistent in-plane biaxial stress — •Senthilnathan Mohanan and Ulrich Herr — Insitut für Mikro- und Nanomaterialien, Universität Ulm, 89081 Ulm

Co/Pd multilayers exhibiting perpendicular magnetic anisotropy (PMA) are promising candidates for perpendicular recording media. In these multilayers, stress induced magnetic anisotropy contributes significantly to the PMA due to the high negative magnetostriction constant. We present a study about the optimization of the magnetic properties of Co/Pd multilayers by changing the magnetoelastic contribution to the anisotropy energy [1]. An in-plane biaxial tensile stress was applied to the Co/Pd multilayers by loading the Ta substrate with hydrogen. In-situ x-ray analysis during hydrogen loading and unloading showed that the hydrogen can absorb and desorb from the Co/Pd multiplayer under the conditions used, but that it remains in the Ta substrate after exposing the sample to air again. This leads to a persistent in-plane biaxial stress of up to 2.8 GPa in the Co/Pd mulilayers. We observed an increase of Hc and the remanent magnetization with increasing biaxial stress. Analysis of the effective perpendicular anisotropy Keff in terms of a simple model yields the corresponding magnetostriction constants. The authors gratefully acknowledge financial support by the Landesstiftung Baden-Württemberg, Germany.

1. S. Mohanan, and U. Herr, J. Appl. Phys. 102, 93903 (2007)

MM 41.9 Thu 18:00 Poster B

Remote control of the Fe magnetic moment in magnetic heterostructures — •Arndt Remhof[1,2], Gregor Nowak[1], Hartmut Zabel[1], Matts Björck[3], Martin Pärnaste[3], Björgvin Hjörvarsson[3], and Valery Uzdin[4] — [1]Department of Physics, Ruhr-Universität, Bochum, Germany — [2]Empa, Swiss Federal Laboratories for Materials Research, Dübendorf, Switzerland — [3]Department of Physics, Uppsala University, Sweden — [4]Saint-Petersburg State Uni-

versity, Russia

In magnetic superlattices with interlayer exchange coupling, not only the coupling strength but also the magnetic moment of the ferromagnetic layer can be altered non-locally by modifying the electronic structure of the non-magnetic spacer layer. Specifically, changes of the electronic structure of the V spacer layers in Fe/V (001) superlattices are seen to affect the adjacent Fe layers. By reversibly loading the V layer with hydrogen, the magnetic moment of Fe increases, whereas the induced magnetic moment in V remains unchanged. The nature of this remote and non-local control of the magnetic moment is connected with a d-electron charge transfer and effective shift of the Fermi level relative to the d-bands of Fe and V, as elucidated on the basis of self-consistent electronic structure calculations [1].

We acknowledge financial support of the DFG under contract RE 2203-1/1, DFG - RFBR project 06-02-04005, INTAS-NETWORK project (03-51-4778) and from VR, the Swedish research council.

[1] A. Remhof et al, Europhys. Lett, 79 37003 (2007).

MM 41.10 Thu 18:00 Poster B

High pressure techniques for synthesis and characterization of hydrogen storage materials — •Carine Rongeat, Isabel Llamas Jansa, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

High pressure reactive milling is a very effective synthesis technique for hydrogen storage materials. It was used successfully to synthesize light metal hydride by milling metal powder under high hydrogen pressure [1]. This technique can also be applied to the synthesis of novel promising complex hydrides. For example, one-step synthesis of doped-sodium alanate was performed from NaH, Al and 4

[1] Doppiu et al., J. Alloys Compd. 427 (2007) 204-208.
[2] Rongeat et al., J. Phys. Chem. B (2007) accepted.

MM 41.11 Thu 18:00 Poster B

Formation and Hydrogen Reactivity of Complex Mg-Ni-La-(Co)-H phases — •Angelika Teresiak, Annett Gebert, Valentin Bunea, Jürgen Thomas, Jürgen Eckert, and Ludwig Schultz — Leibniz Institute for Solid State and Material Research Dresden,

Currently, $Mg * Ni * RE(La)$ alloys are of great interest as new electrode materials for Ni-MH batteries. The recently discovered Mg_2NiLaH_7 hydride in the $Mg - Ni - La - H$ quaternary system shows with 2,8 wt% (109 g/l H) a much higher hydrogen content than the well-known commercial $LaNi_5H_x$- and TiV_2H_x alloys.
In the present study we investigate the formation of the complex hydride $Mg_2NiLa(Co)H_{7*x}$ by using various process routes, which aim at achieving material with nanocrystalline microstructure. The Mg_2NiLaH_7 forms completely by intensive ball milling of an inductively molten master alloy of Mg_2NiLa under hydrogen for 7.5h. Also, the gradual electrolytic charging of the master alloy using a current density of $-1mA/cm^2$ succeeded in forming the hydride. Starting from melt-spun amorphous ribbons, the crystallisation to nanocrystalline Mg_2NiLa and a subsequent hydrogenation under 0.5MPa hydrogen for 26h were performed and monitored by means of in situ high temperature XRD. Furthermore, the influence of Co additives to Mg_2NiLa on the phase formation and hydrogen absorption processes was studied.

MM 41.12 Thu 18:00 Poster B

The role of hydrogen in the development of free-machining titanium alloys — Carsten Siemers, Martin Bäker, •Hans-Rainer Sinning, and Joachim Rösler — Institut für Werkstoffe, TU Braunschweig, Langer Kamp 8, 38106 Braunschweig

Recently considerable effort has been made to improve the poor machinability of titanium and titanium alloys like Ti6Al4V. One of different possibilities is the use of hydrogen as a temporary alloying element: specimens are etched to remove surface layers, and heat treated in hydrogen atmosphere at 600-850°C to charge the Ti matrix with hydrogen (ca. 10-20 at%). Cutting operations are performed in the hydrogen-loaded state, which reduces the cutting force progressively with increasing cutting speed, up to 50% under high-speed cutting (up to 100 m/s) conditions. Finally, the hydrogen is removed from the samples by a heat treatment in vacuum, to restore the mechanical properties of the original alloy.

Such H-induced reduction of the cutting force can be attributed to two effects: the stabilisation of the high-temperature bcc β phase of titanium, which is softer and more ductile than the hcp α phase, and the so-called HELP (hydrogen-enhanced local plasticity) mechanism. The latter results from the shielding of the elastic interaction between dislocations and obstacles due to hydrogen moving along with the dislocations, which eases the shear deformation in the cutting zone where the temperatures exceed 200°C. The effect becomes more pronounced at higher cutting speed, with higher local temperatures and therefore faster hydrogen diffusion in the cutting zone.

MM 41.13 Thu 18:00 Poster B

Microstructure and electrical conductivity of Cu-Ti alloys aged in hydrogen atmosphere — •Satoshi Semboshi[1,2], Ryota Gemma[2], Talaat Al-kassab[2], Astrid Pundt[2], and Reiner Kirchheim[2] — [1]Materials Science and Engineering, Osaka Prefecture University — [2]Institut für Materialphysiks, Uni. Göttingen

The influence of the aging in a hydrogen atmosphere on the electrical properties of Cu-1 and 3 at. % Ti alloys was investigated by means of electrical conductivity measurements and structural measurements using the X-ray diffraction, transmission electron microscopy and atom probe tomography. In the Cu-3 at.%Ti alloy, aging for 48 hours at 773 K in hydrogen atmosphere leads to an improvement of the electrical conductivity up to 65 % IACS (International Annealed Copper Standard), in comparison the value obtained for the alloy aged in a vacuum atmosphere. In addition, aging in hydrogen atmosphere leads to an efficient decrease of the lattice parameter of the Cu solid solution (Cuss) phase, suggesting a significant decrease of the Ti concentration in the Cuss phase. An important structural finding is the existence of not only a needle-shaped Cu$_4$Ti phase but also some cuboidal TiH$_2$ phase precipitates in the alloy aged in the hydrogen atmosphere. We, therefore, conclude that the aging in a hydrogen atmosphere strongly promotes the depletion of Ti in the Cuss phase because of the Cu$_4$Ti and TiH$_2$ precipitates formation, resulting in the significant improvement of the electrical conductivity. This work is partly supported by Inamori Foundation in Japan.

MM 41.14 Thu 18:00 Poster B

First principles analysis of Hydrogen in Manganese-rich austenitic steels — •Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Austenitic Mn-rich steels denote a promising new class of steels, since they combine high strength with ductility. Like other high strength steels, however, they are highly sensitive to hydrogen embrittlement (HE). Various microscopic mechanisms have been discussed as source of HE but the dominant mechanism has not been resolved so far. For a quantitative understanding a description of thermodynamic as well as kinetic aspects of the hydrogen-steel interaction is essential. We have therefore employed density functional theory to investigate the solubility and mobility of interstitial H in the austenitic phase of Fe, Mn, and Fe(x)Mn(1-x). For Fe(x)Mn(1-x) in the paramagnetic state our results show a significant increase both in the solubility and mobility of the H impurity with increasing Mn concentration. A detailed analysis shows that this effect is exclusively related to larger lattice volume induced by Mn. In addition we investigated the interaction of H with interstitial carbon. Our results show that at the high C-concentrations characteristic for the Mn steels the H solubility and mobility increase. This effect is caused by an (anisotropic) volume expansion of the lattice.

MM 41.15 Thu 18:00 Poster B

In-situ deformation study of porous nanocrystalline Pd during electrochemical charging — •Viswanath Raghavan Nadar[1], Dominik Kramer[1], and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Technische Physik, Universität des Saarlandes, Saarbrücken, Germany

The length of porous nanocrystalline palladium in a nearly neutral aqueous NaF (0.7 M) electrolyte was measured using a commercial dilatometer as a function of the applied electrode potential and of the charge. As expected, the sample expands during formation of the palladium hydride phases. However, the length is not just a simple function of the faradaic charge, but shows a remarkable fine structure which we discuss using a comparison with other nanoporous samples, e.g. gold and platinum. Even without hydrogen ad- or absorption, the length of nanometals varies as a function of charge due to the variation of surface stress with charge density, which causes large variations of the bulk pressure of nanomaterials due to their large ratio of the number of surface atoms relative to the number of bulk atoms. The surface stress behaviour of palladium observed at potentials positive of the hydrogen adsorption is qualitatively similar to that of porous

platinum, although there is a quantitative difference if one relates the expansion to the charge density, e.g. by calculating the surface stress-charge coefficient. The highly reproducible cyclic strain caused by hydrogen absorption and -desorption in Pd is larger than the surface stress effects by more than an order of magnitude.

MM 41.16 Thu 18:00 Poster B

Absolutbestimmung der Wasserstoffkonzentration innerhalb der plastischen Zone der Aluminiumlegierung AA6013 — •Christian Lenk, Thorsten Loewenhoff, Matz Haaks und Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, D-53115 Bonn, Germany

In ersten ortsaufgelösten Messungen an einer wechselverformten CT-Probe aus der Legierung AA6013 konnte bereits eine erhöhte Wasserstoffkonzentration in der plastischen Zone vor der Rissspitze nachgewiesen werden. Findet die Wechselverformung in einer korrosiven Umgebung statt, so dass Wasserstoff in die Probe diffundieren kann, führt dies zu einer erhöhten Rissausbreitungsgeschwindigkeit und einem verzögerten Ausheilverhalten von Fehlstellen in der plastischen Zone. Der Nachweis erfolgt dadurch, dass im UHV Späne mit einer Dicke von wenigen μm aus einer Probe herausgesägt und in situ ausgeheizt werden. Der folgende Anstieg des Partialdrucks wird mit einem Massenspektrometer aufgenommen. Es wird eine Methode vorgestellt, mit der es möglich ist, die absolute Wasserstoffkonzentration im Span aus der plastischen Zone zu bestimmen.

MM 41.17 Thu 18:00 Poster B

Hydrogen in ZnO - a challenge to experiments and theory — •Gerhard Brauer[1] and Jan Kuriplach[2] — [1]Forschungszentrum Dresden-Rossendorf e.V., Dresden, Germany — [2]Charles University, Prague, Czech Republic

Positron lifetime spectroscopy, nuclear reaction analysis and X-ray diffraction have been combined to investigate various, nominally undoped, ZnO single crystals. Hydrogen is detected in all crystals in a bound state (0.3 - 0.8 at.-%), and in some cases also in an unbound state (0.7 * 1.9 at.-%), which can be removed by annealing. A single positron lifetime of 180-182 ps and 165-167 ps is measured for all hydrothermally and melt grown crystals, respectively. These lifetimes are attributed to zinc vacancy-hydrogen complexes, as deduced from ab initio studies of various vacancy-hydrogen defect configurations in ZnO and related positron calculations. In addition, various defect studies of hydrothermally grown (0001) oriented ZnO crystals electrochemically doped with hydrogen are presented. It is demonstrated that a very high amount of hydrogen (up to ˜30 at.-%) can be introduced into the crystals by electrochemical doping. It is found that more than half of this amount is chemically bound, i.e. incorporated into the ZnO crystal lattice.

MM 41.18 Thu 18:00 Poster B

Hydrogen in V-8at%Fe single-layered films and Fe/V multi-layered films — •Ryota Gemma, Talaat Al-Kassab, Reiner Kirchheim, and Astrid Pundt — Institut fuer Materialphysik, Friedrich-Hund-Platz 1, D-37077, Goettingen, Germany

The influence of out-of-plane lattice parameter a_0 of V layer on the plateau slope of electromotive force (EMF) curves of V-8at%Fe films and Fe/V multi-layered films was investigated by applying in-situ XRD and in-situ stress measurements equipped with electrochemical hydrogen loading set up. For the films with small a_0, the plateau slope and hydrogen-induced stress were found to be larger than those with larger a_0. This trend can be qualitatively understood if we consider that hydrogen atoms predominantly occupy O_z sites in vanadium hydride phase, unlikely for the materials with isotropic site occupation as Pd. The deuterium distribution in the same kind of (110) films was also investigated by atom probe tomographic analysis (APT). The depth profile of the Fe/V films showed D atoms concentrated in V layers, as expected from the fact that V has bigger enthalpy for hydrogenation than that of Fe. However, the D concentration was not homogeneous in a V layer and far below the expected value from EMF curve. A similar phenomenon was found also for V-8at%Fe single-layered film. The results will be discussed in terms of difference in the microstructure and initial stress of the films.

MM 41.19 Thu 18:00 Poster B

Wechselverformungsmaschine für spezielle Anforderungen — •Thorsten Loewenhoff, Christian Lenk, Matz Haaks und Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, D-53115 Bonn, Germany

Zur Untersuchung dünnwandiger Al-Legierungen für den Flugzeugbau wurde eine Wechselverformungsmaschine konstruiert, um den speziellen Anforderung an die Probendimensionen zu genügen. Der Aufbau erlaubt mittels einer Piezokeramik Wechselverformungen im Bereich von einigen 10 μm Amplitude mit Frequenzen von 0,1 Hz bis 50 Hz. Die entwickelte Steuerungssoftware stellt verschiedene Signalformen (Sinus, Dreieck, Rechteck) zur Verfügung und nimmt Daten (Kraft auf die Probe, Verformungsamplitude) zur späteren Analyse auf. Im Gegensatz zu hydraulischen Verformungsmaschinen lässt die Piezokeramik Rechtecksignale mit guter Flankensteilheit zu. Dies ermöglicht Untersuchungen der Eindiffusion von Wasserstoff an Rissspitzen in Al-Legierungen.

MM 42: Phase Transitions III

Time: Thursday 14:00–15:30 Location: H 0107

MM 42.1 Thu 14:00 H 0107

Stress Induced Martensite in Epitaxial Ni-Mn-Ga Films — •Michael Thomas[1,2], Jörg Buschbeck[1], Oleg Heczko[1], Ludwig Schultz[1,2], and Sebastian Fähler[1,2] — [1]IFW Dresden, P.O. Box: 270116, 01171 Dresden, Germany — [2]Institute for Solid State Physics, Department of Physics, Dresden University of Technology, 01062 Dresden, Germany

Martensitic epitaxial Ni-Mn-Ga films with a thickness of about 500 nm were deposited at different temperatures on MgO(001) substrates. Some films are in an orthorhombic martensite state at room temperature though their compositions suggest far lower martensitic transformation temperatures. The martensite transformation is stress induced which was confirmed by X-ray stress analysis. The film structure can be explained as having an austenite layer at the interface between film and substrate. A hierarchical twinned martensite phase is grown on this austenite layer separated by a (101)-habit plane. The distribution of the twin boundaries is controlled by the stress state arising from the substrate constraint. Additionally non-modulated Ni-Mn-Ga films with a tetragonal phase and a coexisting cubic austenite phase were grown. Peeling this films off the substrate leads to the vanishing of the residual austenite phase. The strongly acting stress during the peeling may induce a fully tetragonal non-modulated martensite phase.

MM 42.2 Thu 14:15 H 0107

Microstructure and mechanical properties of sputter deposited NiMnGa magnetic shape memory alloy thin films — •Guido J. Mahnke and S. G. Mayr — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

While bulk magnetic shape memory alloys (MSMA) are well established - and even commerically available, miniaturization as thin functional films still remains an open issue. The relation of microstructure and mechanical properties is one of the key ingredients to understand the martensitic transformation behaviour as well as twin boundary movement in MSMA thin films. To achieve this, highly textured and epitaxial NiMnGa MSMA thin films were preprared on different substrates at variable temperature by ion beam sputtering from a multicomponent target, and charcterized with respect to phase, microstructure and growth stresses. While growth usully occurred in the austenitic phase, a twinned martensitic state usually could be obtained during cooling down, accompanied by changes in the stress state. The relation of mechanical properties and microstructure is discussed.

This project is funded by the DFG priority programme 1239, Project C4.

MM 42.3 Thu 14:30 H 0107

Growth of epitaxial and highly textured FePd shape memory alloy thin films — •Lisa Kühnemund, Tobias Edler, and S.G.

Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Thin films of the MSM alloy $Fe_{70}Pd_{30}$ are grown by e-beam evaporation. In order to achieve a maximum strain by the MSM effect, epitaxial or highly textured films are desirable. Depending on the substrate type (either MgO single crystals or amorphous SiO_2) key properties, including phase, microstructure, and magnetic characteristics have been determined. Since the stress state of a thin film is known to have a major influence not only on the matensitic transformation but also on the MSM effect itself, stress measurements on films grown by e-beam evaporation are compared to films grown by PLD. In order to influence the texture of polycrystalline films, methods of applying a magnetic field both during film growth and post-deposition annealing are evaluated. The implications of these structural and magnetic properties on the MSM effect and its possible applications are discussed.

This work has been financially supported by the DFG-SPP 1239, Project C4.

MM 42.4 Thu 14:45 H 0107

Intrinsic Properties and Growth of Iron Palladium Thin Films — •Iris Kock and S.G. Mayr — 1. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Iron Palladium alloys of a composition around $Fe_{70}Pd_{30}$ are among the most promising candidates for magnetic shape memory alloys. With regard to possible application in miniaturized devices the intrinsic properties of thin films prepared by electron beam evaporation were investigated and compared to those of splat quenched foils. The developement of mechanical stress and surface morphology during film growth were studied and linked to crystal structure, microstructure and magnetic properties to determine the growth mechanisms. It was found that deposition at room temperature leads to films in a bct structure with an out of plane magnetization. Transformation to the fcc austenite phase can be achieved by appropriate heat treatment. Splat quenching directly yields foils of about 60 microns thickness in the austenite phase that can transform into the martensite phase upon cooling.

Financial support by DFG SPP1239 TP C4 is gratefully acknowledged.

MM 42.5 Thu 15:00 H 0107

Structural, magnetic and phase transformation properties of Fe-Pd-X thin films — •Sven Hamann[1,2], Sigurd Thienhaus[1,2], Alan Savan[1], and Alfred Ludwig[1,2] — [1]Combinatorial Materials Science Group, Center of Advanced European Studies and Research (Caesar), Ludwig-Erhard-Allee 2, 53175 Bonn, Germany — [2]Institute for Materials, Faculty of Mechanical Engineering, Ruhr-University Bochum, 44780 Bochum, Germany

The topic of this work is the development of new ferromagnetic shape memory alloys (FSMA) within the Fe-Pd-X system (X=Co, Mn,...) with improved intrinsic properties (high transformation temperatures [MS > 100°C], high Curie temperature and high magnetocrystalline anisotropy). The advantages of Fe70 Pd30-based FSMA in comparison to Ni-Mn-Ga are higher Curie temperatures, saturation magnetization and transformation temperatures as well as potentially higher magnetocrystalline anisotropy. The Fe-Pd-X thin films were fabricated by co-sputtering from different elemental targets in a combinatorial magnetron sputter system. This method is used to create over 300 samples with different compositions on a 4" wafer substrate in one deposition process. The annealed Fe-Pd-X thin films were characterized by energy dispersive x-ray spectroscopy, electrical resistance versus temperature measurements, x-ray diffraction, vibrating sample magnetometry measurements and transmission electron microscopy. Results from several new Fe-Pd-X systems are presented, which show martensitic transformation temperatures above 100°C.

MM 42.6 Thu 15:15 H 0107

Microstructure of epitaxial films of the magnetic shape memory alloy Ni_2MnGa — •Tobias Eichhorn, Michael Kallmayer, Hans-Joachim Elmers, and Gerhard Jakob — Institut für Physik, Universität Mainz, Staudinger Weg 7, 55099 Mainz

Since the first discovery of the magnetic shape memory effect by Ullako et al. interest in this material group has increased continuously. By application of a magnetic field, length changes up to 10 % can be achieved in single crystals of martensitic Ni_2MnGa. However the microscopic mechanism is far from being completely understood. To improve this understanding, single crystalline thin films allow elaborate measuring techniques and form the basis for development of applications on a small length scale.

Thin epitaxial films of Ni_2MnGa and $Ni_{1.96}Mn_{1.22}Ga_{0.82}$ are grown by dc-magnetron sputtering onto heated $Al_2O_3(11\bar{2}0)$ and $MgO(100)$ substrates. To investigate the structural and magnetic properties of the samples we use temperature dependent x-ray diffraction and magnetometry. To get insight on microscopic magnetism and electronic structure x-ray absorption spectroscopy and magnetic circular dichroism measurements have been performed at the German synchrotron light source BESSY II (Berlin). Concerning technological applications free-standing single crystalline films will be needed. For that purpose water-soluble substrates and suitable sacrificial layers are investigated. To detect the magnetically induced shape memory effect in our films without removal of the substrate we build a setup to measure the magnetostriction by a capacitive method.

MM 43: Phase Transitions IV

Time: Thursday 16:00–17:15 Location: H 0107

MM 43.1 Thu 16:00 H 0107

Effect of composition and heat treatment on martensitic transformation and magnetic properties in Ni-Fe-Ga-Co magnetic shape memory alloys — •Jian Liu, Nils Scheerbaum, Dietrich Hinz, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

Ni-Fe-Ga-Co is a promising alloy system for magnetic shape memory alloy applications, due to its good ductility, mobile twin boundaries and high transformation temperatures. Here, the martensitic transformation and magnetic properties in a large composition range with Ni54-xFe20Ga26Cox, Ni54-xFe19Ga27Cox, Ni56-xFe17Ga27Cox and Ni54-xFe18Ga28Cox (x = 0, 2, 4) are investigated. The martensitic transformation temperature Tm and the Curie temperature Tc can be tailored in a wide range by changing composition and heat treatment (ageing temperature, time and cooling rate), Tm ˜ -100 to 100 C and Tc ˜ 10 to 130 °C. A coupling of martensitic and magnetic transformations at a relatively high temperature (˜ 90 °C) is found for Ni52Fe17Ga27Co4. In this composition, increasing the degree of atomic order by long ageing and slow cooling decreases Tm but keeps Tc unchanged. Compared to ageing at 300 °C, after ageing at 400 °C there is no obvious change in Tm and Tc, but the transformation hysteresis is increased and the transformation interval is decreased significantly. However, the presence of γ precipitates induced by ageing at 500 °C suppresses the occurrence of the martensitic transformation itself.

MM 43.2 Thu 16:15 H 0107

First-principles study of hexagonal to cubic phase transformations in Laves phases $NbCr_2$ and $TaCr_2$ — •Olena Vedmedenko[1], Frohmut Rösch[1], and Christian Elsässer[2] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — [2]Fraunhofer-Institut für Werkstoffmechanik, Wöhlerstr. 11, 79108 Freiburg

The Laves phases $NbCr_2$ and $TaCr_2$ are two technically attractive intermetallic compounds with high melting temperature, high oxidation resistance, and low density. The thermodynamically most stable phases of both are hexagonal (C14) at high temperatures and cubic (C15) at low temperatures. However, the kinetics of the phase transformations leads to significantly different microstructures. To get a deeper scientific understanding of their evolution from the atomic scale, we have systematically studied the hexagonal to cubic phase transformations with respect to a synchroshear deformation mechanism. Total energies of structurally optimised atomistic supercell models have been calculated from first principles, by means of density functional theory with the local density approximation and a mixed-basis pseudopotential method. We obtain a quantitative description of activation energy

profiles for deformation paths from hexagonal (high-temperature) to cubic or twinned cubic (low-temperature) phases. Based on these activation energy profiles we discuss differences in the transformation behaviour and interpret recently reported experimental observations of microstructural features for the two compounds.

MM 43.3 Thu 16:30 H 0107

Genuine Metal-Insulator Transition of V_2O_3 Revealed by Hard X-ray Photoemission — •Hidenori Fujiwara[1,2], Akira Sekiyama[1], Junnichi Yamaguchi[1], Gen Funabashi[1], Shin Imada[1], Sung-Kwan Mo[3,4], James W. Allen[3], Patricia Metcalf[5], Atsushi Higashiya[6], Makina Yabashi[7], Kenji Tamasaku[6], Tetsuya Ishikawa[6,7], and Shigemasa Suga[1] — [1]Graduate School of Engineering Science, Osaka University, Toyonaka, Japan — [2]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [3]Randall Laboratory of Physics, University of Michigan, Ann Arbor, USA — [4]Department of Physics, Stanford University, Stanford, USA — [5]Department of Physics, Purdue University, West Lafayette, USA — [6]SPring-8/RIKEN, Sayo, Japan — [7]SPring-8/JASRI, Sayo, Japan

V_2O_3 is a paradigmatic example of Mott-Hubbard (MH) metal-insulator transition (MIT) materials; it displays the 1st-order transition from the paramagnetic metal (PM) to the antiferromagnetic insulator (AFI) at 150 K. In order to reveal the mechanism of the Mott-Hubbard metal-insulator transition (MH-MIT) in V_2O_3, we have performed the hard X-ray photoemission (HAXPES) with $h\nu = 8170$ eV at BL19LXU in SPring-8. The energy resolution was set to 130 meV. The clean surface of the single crystalline sample was obtained by cleavage in situ in ultra-high vacuum. The significant spectral transfer of the V 3*d* states is observed through the MH-MIT. We reveal the simple Mott-Hubbard scenario does not describe the transition, and new reliable model is required to explain"the MH-MIT on V_2O_3.

MM 43.4 Thu 16:45 H 0107

Photoinduced ultrafast volume changes in intermediate valence solids — •momar diakhate and martin garcia — Institut für Physik, Universität Kassel, D-34132 Kassel, Germany

We present a theoretical model for the description of the ultrafast structural response of intermediate valence solids to femtosecond laser excitation. Based on the promotional Ramirez-Falicov model we consider the femtosecond laser heating of γ Cerium and the subsequent ultrafast lattice expansion dynamics.

In particular we determine the thermodynamic and electronic properties of cerium metal at very high electronic temperatures (simulating the laser excitation). The possibility for a non-equilibrium photoinduced inverse volume collapse transition is discussed. The p-v-T equation of state is obtained from the Helmoltz free energy in the usual way of thermodynamic derivatives by considering an adiabatic expansion of the crystal at high temperature.

We take into account both the laser excited and the unexcited parts of the system, in oder to account for inertial confinement. The thermodynamic properties were obtained as function of time and used to calculate the shock velocity variation and in the surrounding (unheated) part of the sample.

MM 43.5 Thu 17:00 H 0107

An *ab-initio* study of the phase transitions in the interstitial Fe-C solid solutions — •Alexander Udyansky, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 402 37, Düsseldorf, Germany

The Fe-C system constitutes the backbone of the steel industry that has long been altering our daily life. The Fe-C phase diagram is very rich in different phases exhibiting both low-carbon concentration, like ferrite or martensite, and high-carbon content, as e.g. austenite or cementite. An important prerequisite for the nucleation and formation of the latter is the existence of regions in the Fe matrix with diffusion-enhanced carbon concentration. In order to gain a detailed insight into properties of the high-C regions we have theoretically determined the formation energies, magnetic moments, and structural properties of selected interstitial Fe-C solid solutions employing density functional theory (DFT) in the generalized gradient approximation (GGA). The interstitial solid solutions have been modeled using the super-cell approach. Both magnetic and structural phase transformations induced by increasing carbon concentration are predicted and the very strong interplay between the C-content and both structural and magnetic degrees of freedom is found and analyzed.

MM 44: Bioinspired Materials

Time: Thursday 14:00–14:30 Location: H 0111

MM 44.1 Thu 14:00 H 0111

AFM-investigation of differently treated Ti-surfaces with respect to their usability for dental implants — •Sebastian Wille[1], Bin Yang[2], Rainer Adelung[1], and Birte Grössner-Schreiber[3] — [1]Funktionale Nanomaterialien, Institut für Materialwissenschaft, CAU Kiel Kaiserstr. 2 24143 Kiel — [2]Klinik für Zahnärztliche Prothetik, Propädeutik und Werkstoffkunde, Arnold-Heller-Strasse 16, 24105 Kiel — [3]Klinik für Zahnerhaltungskunde und Parodontologie, Arnold-Heller-Str. 16, 24105 Kiel

Microbial adherence to dental implant surfaces is one initiating step in the formation of plaque and is considered to be an important event in the pathogenesis of peri-implant disease [1]. Besides good connective tissue adhesion in the transmucosal part of an implant, titanium implants exposed to the oral cavity require surface modification to inhibit the adherence of oral bacteria. Surface roughness and chemical composition of the implant surface were found to have a significant impact on plaque formation. The aim of the present study was to examine bacterial adherence of differently modified potential implant surfaces. Therefore the surface roughness was decreased and for example a thin ceramic or composite layer of antibacterial material was deposited on abutment surface by sputtering. We analyze the new surface with AFM to control the roughness. For further characterization contact angle measurements were carried out. Biocompatibility and antibacterial effects will be determined in cooperation with the dental clinic at the University Kiel.

[1] B. Größner-Schreiber et al. Clin Oral Impl Res 12, 543-551 (2001)

MM 44.2 Thu 14:15 H 0111

Mechanical implications of the inhomogeneity of bone material — •Carolin Lukas[1,2], Davide Ruffoni[1], Peter Fratzl[1], Paul Roschger[3], Klaus Klaushofer[3], and Richard Weinkamer[1] — [1]Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany — [2]TU Berlin, Germany — [3]Ludwig Boltzmann Institute of Osteology, Vienna, Austria

The mechanical behaviour of bone at the material level is determined by the amount and the distribution of mineral. Bone mineral is heterogeneously distributed because of the continuous remodeling of bone and the consecutive mineralization process. During bone mineralization each newly deposited bone packet increases its stiffness by increasing its mineral content. Differences in mineral content are experimentally accessible and are characterized by a frequency distribution of the mineral content called the bone mineralization density distribution (BMDD). A mathematical framework was developed to predict how different remodeling rates result in different BMDDs. The mechanical implications of such mineralization distributions are here investigated. First, combining measurement of mineral content with micromechanical tests, the BMDD is converted into a distribution of elastic moduli. Secondly, assuming an ideal geometrical arrangement of the bone packets inside the trabeculae the bounds for the elastic properties are established for the different material distributions. Considering then more realistic 3D arrangements of the bone packets, the mechanical implications of the different types of BMDD are computed at the trabecular level.

MM 45: Nanostructured Materials VI

Time: Thursday 15:00–16:00 Location: H 0111

MM 45.1 Thu 15:00 H 0111

Analysis of sorption strains in mesoporous silica by in-situ x-ray diffraction — •Johannes Prass, Dirk Müter, John Dunlop, Stefan Siegel, Chenghao Li, and Oskar Paris — Max Plank Institut für Kolloid und Grenzflächenforschung, 14424 Potsdam, Germany

Sorption and capillary condensation of fluids in ordered mesoporous silica (SBA-15 and MCM-41) were studied by in situ small-angle X-ray diffraction using synchrotron radiation. Diffraction peaks resulting from the pore lattice were evaluated in terms of lattice strains. Intensity, position and width of the diffraction peaks show pronounced changes in the capillary condensation/evaporation regime. At complete pore filling, an expansion of the lattice is observed which can be explained by the decrease of total interfacial energy. A contraction of the pore lattice is observed for the nearly filled pores for both branches of the sorption isotherm, which is attributed to liquid menisci due to capillary condensation of fluid in the pores. Data measured for fluids with different surface tension and silica materials with different pore width allow to vary elastic strains in the pore lattice and to compare them with simple models.

MM 45.2 Thu 15:15 H 0111

Modeling experimental SAXS data from fluid sorption in ordered mesoporous silica — •Dirk Müter[1], Susanne Jähnert[2], Gerhard Findenegg[2], and Oskar Paris[1] — [1]Department of Biomaterials, MPI of Colloids and Interfaces, Potsdam — [2]Stranski Laboratory of Physical and Theoretical Chemistry, TU Berlin

Experimental small angle x-ray scattering (SAXS) data from an in-situ sorption experiment of dibromomethane (CH_2Br_2) in 2D hexagonally ordered mesoporous silica (SBA-15) are evaluated using two complementing modeling approaches. The SAXS data were measured as a function of relative vapor pressure of dibromomethane at room temperature. The integrated intensities of up to 10 measured Bragg reflections were simultaneously fitted with a superposition of analytical functions derived from an improved model for the formfactor of the pore/liquid system [1]. By this the pore morphology can be described, and the sorption process can be followed quantitatively in terms of liquid film formation and capillary condensation. However, a discrepancy of the total amount adsorbed is noticed in comparison to the sorption isotherm measured by a microbalance. To account for this difference we have studied a model in which additional micropores are randomly inserted in the mesopore walls of the silica matrix. Numerical Fourier transformation of this model system shows that the micropores contribute mainly to diffuse scattering while adsorption into these additional pores improves the agreement with the microbalance measurements.

[1] G. Zickler et al., Phys. Rev. B 73 (2006) 184109.

MM 45.3 Thu 15:30 H 0111

Elastic properties of argon adsorbed in nanoporous glass — •Klaus Schappert and Rolf Pelster — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus E 2.6, D-66123 Saarbrücken

We have performed isothermal adsorption and desorption experiments on argon in nanoporous Vycor. The effective shear modulus has been determined measuring the amount of absorbed argon as well as the ultrasonic velocity near 12.5 MHz. Since fluids cannot sustain shear stress, argon only affects the effective shear modulus at temperatures below its freezing point ($T_{f,conf} < T_{f,bulk}$). Depending on the filling fraction, three different behaviours are observed: (i) The first adsorbed argon layers do not contribute to the measured shear modulus. (ii) In an intermediate range the shear modulus increases linearly with increasing argon content. (iii) At a characteristic filling fraction an abrupt enhancement of the shear modulus is observed. We discuss these phenomena in terms of capillary sublimation and crystallization.

MM 45.4 Thu 15:45 H 0111

Li diffusion in nanocrystalline and nanoglassy β-spodumene $LiAlSi_2O_6$ — •Alexander Kuhn, Martin Wilkening, and Paul Heitjans — Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Callinstr. 3-3a, 30167 Hannover

Recently nanocrystalline and nanoglassy ceramics have been a subject of growing research interest. In the present study β-spodumene $LiAlSi_2O_6$ and the corresponding glass were used as a model system. The influence of particle size on Li ion dynamics was studied by ^{7}Li NMR spin-lattice relaxation rate measurements. As a general trend, the Li diffusivity in the glassy sample is larger than that in the μm-sized crystalline material [1, 2]. However, as the particle size decreases, the nanocrystalline material shows enhanced diffusivity whilst the opposite effect is found for the nanoglassy ceramics. The nanocrystalline and nanoglassy samples were prepared by high-energy ball-milling of the coarse grained starting material and the corresponding glass, respectively. A possible structural model trying to explain the observed convergence of the diffusivities of the nanocrystalline and nanoglassy samples is discussed.

[1] F. Qi, C. Rier, R. Böhmer, W. Franke and P. Heitjans, *Phys. Rev. B* **72** (2005) 10430.

[2] W. Franke and P. Heitjans, *Ber. Bunsenges. Phys. Chem.* **96** (1992) 1674.

MM 46: Interfaces

Time: Thursday 16:30–18:15 Location: H 0111

MM 46.1 Thu 16:30 H 0111

Effect of the finite mobility the grain boundary junctions on the MacPherson-Srolovitz relation for the growth rate of polycrystalline systems — •Luis Antonio Barrales Mora[1], Volker Mohles[1], Lasar S. Shvindlerman[1,2], and Günter Gottstein[1] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, D-52074 Aachen, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow District 142432, Russia

Recently, MacPherson and Srolovitz formulated the three-dimensional equivalent to the von Neumann-Mullins relation. In contrast with the latter, the new relation does not include directly the topological class of the grains but relates mainly to their metrics. Since a finite mobility of the boundary junctions (triple lines and quadruple junctions) affects the kinetics of the evolution of the granular system, repercussions in the MacPherson-Srolovitz relation are to be expected. In the present contribution, a three-dimensional vertex model is used in simple granular assemblies for the verification of this important relation. In addition, the effect of a finite mobility of the boundary junctions and its impact on the MacPherson-Srolovitz relation is analysed.

MM 46.2 Thu 16:45 H 0111

Mechanisch induzierte Bewegung der <100> Kippkorngrenzen in Al-Bikristallen — •Tatiana Gorkaya, Dmitri A. Molodov und Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen

Es wurde die Bewegung von planaren Korngrenzen, die durch eine angelegte Schubspannung induziert wurde, in Al-Bikristallen gemessen. Symmetrische <100> Kippkorngrenzen mit Rotationswinkeln im gesamten Desorientierungsbereich (0-90°) wurden dabei untersucht. Die Experimente zeigten ideale Kopplung zwischen der Korngrenzenbewegung in die Richtung normal zur Korngrenzenebene und der lateralen Verschiebung der Körner. Die gemessenen Verhältnisse zwischen denen stimmen perfekt mit der entsprechenden Korngrenzengeometrie überein. Weiterhin wurde ein Übergang von der Korngrenzenbewegung, die mit der Kornverschiebung gekoppelt ist, zum rigiden Kornabgleiten entlang der Korngrenzenebene beobachtet, der von der Temperatur, der angelegten Schubspannung und Korngrenzengeometrie abhängt. Die Experimente zeigten auch, dass sich die Korngrenzen mit θ bis etwa 30° und ab 60° in entgegengesetzte Richtungen bewegen. Für Großwinkelkorngrenzen mit θ im mittleren Winkelbereich (30°-60°) wurde die Korngrenzenbewegung in beide Richtungen,

abhängig von experimentellen Parametern, beobachtet. Die Temperaturabhängigkeit der Korngrenzenbeweglichkeit wurde in einem Temperaturintervall zwischen 280 und 400°C gemessen und entsprechende Aktivierungsparameter der mechanisch induzierten Korngrenzenbewegung wurden bestimmt.

MM 46.3 Thu 17:00 H 0111

Simulation of partial melts with a phase-field model — Jens Becker[1], Britta Nestler[2], and •Frank Wendler[2] — [1]Institute of Geoscience, University of Tübingen, Sigwartstr. 10, 72076 Tübingen, Germany — [2]Institute of Computational Engineering, University of Applied Sciences Karlsruhe, Moltkestr. 30, 76133 Karlsruhe, Germany

Partially molten grain systems are of great interest in engineering (thixoforming, rheocasting) as well as in geology, as they appear in the rock forming layers of the deeper earth's crust. Particularly properties like the growth rate of isolated grains as well as coarsening in grain ensembles are substantially modified after partial melting. We present recent results found by applying our formerly introduced multi phase-field model (a diffuse interface method based on the formulation of a Ginzburg-Landau free energy functional) to partial melts. First, details on the phase-field model and the numerical aspects necessary to treat the enormous computational effort for a large grain system are presented. Secondly, a comparison of normal grain growth in 2D with grain growth in partial molten systems is given. The parabolic growth law and the validity of the von Neumann-Mullins relation for isolated grains are found to hold very well in the case of normal grain growth simulations. Partial melts in contrast show a strongly reduced growth rate. The dependancy on wetting angles, liquid fraction and permeability of the grain structure is highlighted using results in from 2D and 3D simulations. Additionally, the evolution of 'wet' triple points including an orientational dependancy of the surface energy are shown as a first step to clarify the role of anisotropy in partial melts.

MM 46.4 Thu 17:15 H 0111

ELNES at internal metal-oxide interfaces — •Oliver Heckl[1] and Ferdinand Haider[2] — [1]ETH Zürich, Institute of Quantum Electronics, Wolfgang-Pauli-Str. 16, 8093 Zürich — [2]University of Augsburg, Institute of Physics,Universitätsstr. 1 , 86135 Augsburg

The heterophase boundaries between precipitates such as spherical amorphous SiO_2 particles inside a copper matrix as well as crystalline CuO precipitates inside a silver matrix and the surrounding metal matrix are examined with high spatial resolution using a scanning transmission electron microscope (STEM) equipped with an electron energy loss spectrometer (EELS). Typical features of the electron energy loss near-edge fine structure (ELNES) of the oxygen K ionization edge allow to determine the bonding state of oxygen and thus to detect interlayers at the phase boundary. The validity of Kirchheim's structural vacancy model of oxygen segregation at metal-oxide interfaces is verified this way. It predicts that no interfacial accumulation of excess oxygen occurs at the phase boundary of amorphous precipitates. For the Ag-Cu alloy there is the additional degree of freedom for the oxidation value of copper and it can be seen that structural vacancies change the oxidation value at the phase boundary.

MM 46.5 Thu 17:30 H 0111

Ab-initio and atomistic simulation of interfaces in Aluminium — •Thomas Gnielka[1], Peter Gumbsch[1,2], Pim Schravendijk[2], and Christian Elsässer[2] — [1]IZBS, Universität Karlsruhe (TH), Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg

Various macroscopic properties of polycrystalline materials originate from their microstructure, which itself depends on structural and chemical properties of extended defects (dislocations, grain and phase boundaries) at the atomic level. Therefore an important task for a scale-bridging modeling of polycrystalline materials is the coupling of different calculation methods at different size and time scales. In this talk an example for the combination of ab-initio calculations, based on the density functional theory (DFT), and atomistic simulations with empirical interatomic potentials will be addressed. While ab-initio DFT methods can calculate energies with high predictive power but for rather small systems, atomistic simulations with potentials validated with respect to first-principles results make it possible to study materials systems with thousands of atoms at a reasonable compromise of accuracy and efficiency. In this work grain boundaries in aluminum were studied as model systems, and first results for two pure boundaries will be presented and discussed.

MM 46.6 Thu 17:45 H 0111

Ab-initio investigation of chromium carbide - diamond interfaces — Andreas Böhner, •Rebecca Janisch, and Alexander Hartmaier — Friedrich-Alexander-University Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute of General Materials Properties

Superhard carbon coatings, e.g. diamond like carbon on ductile tool steels, promise to feature exceptional resistance to frictional wear and corrosion. Therefore, the development of such carbon coatings is an active field of materials research. A crucial task is to optimize the adhesion between the carbon coating and the subjacent alloy.

To this end we perform a case study of the interface between diamond and chromium carbides of different stoichiometry. We use ab - initio density functional calculations employing plane waves and pseudopotentials. The first step is to study bulk properties - such as equilibrium lattice constant, bulk modulus, and details of the chemical bonding - of different chromium carbides. We then select certain phases for constructing supercells to model the CrC_x diamond interface. After relaxing macroscopic and microscopic degrees of freedom, these interfaces are characterized by calculations of the work of separation and investigation of the electronic structure at the boundary. The influence of superimposed stresses and strain on the results is discussed. The results show a systematic dependence of the characteristic quantities on the C concentration in the carbide and can explain different experimental observations.

MM 46.7 Thu 18:00 H 0111

Gaussian Polarizable Model for Metal Oxides — •Fawzi Mohamed and Joachim Sauer — Humboldt University

We present the first results of a polarizable force field geared toward metal oxides which is well suited for QM:MM embedding.

The model uses atom centered gaussians s and p functions to describe the long range electrostatic part.

The s function charge is assumed to be constant (no charge transfer allowed) and the p functions depend on the field and the local environment around each atom.

The optimal values for the s and p functions, the values that the potential tries to fit, are obtained from the electronic density ρ of DFT calculations minimizing

$$E = (\rho - \tilde{\rho}|\rho - \tilde{\rho}) = \int \frac{(\rho(r) - \tilde{\rho}(r))(\rho(r') - \tilde{\rho}(r'))}{|r - r'|} dr dr' \quad (1)$$

as is done in RI methods, but only to reproduce the long range part of it. This is achieved by replacing the $1/|r - r'|$ operator with

$$C(r, r'')F(r'')C(r'', r) \quad (2)$$

where C is half coulomb operator

$$\frac{1}{|r - r'|} = \int C(r, r'')C(r'', r')dr'' \quad (3)$$

and F is a filter that removes the core region of the atoms.

Fitting these optimal values gives an implicitly interacting polarizable model that reproduces well the long range electrostatic field.

Then the short range part of the forcefield is optimized with force matching against DFT results.

MM 47: SYM Hydrogen in Materials: New Developments V

Time: Friday 10:15–11:55 Location: H 1058

MM 47.1 Fri 10:15 H 1058

Mechanisms and thermodynamics of hydrogen embrittlement in metals — •Reiner Kirchheim — Institute for Materials Physics, University of Goettingen, Germany

Depending on temperature, hydrogen concentration, its diffusion coefficient and its terminal solubility different mechanisms of hydrogen embrittlement are relevant. Some of them are dealing with the ease of generating new surfaces (cracks) or dislocations in the presence of hydrogen. The formation energy of these defects as well as their mobility depends on the chemical potential of hydrogen. This relationship is

discussed in the framework of a generalized Gibbs adsorption theory.

MM 47.2 Fri 10:35 H 1058

Hydrogen embrittlement revisited by in-situ electrochemical nanoindentation — •Afrooz Barnoush and Horst Vehoff — Saarland University Bldg. D22 P.O. Box 151150, Postcode D-66041, Saarbruecken, Germany

Electrochemical NI-AFM was used to examine the effect of hydrogen on dislocation nucleation. It was shown that hydrogen reduces the pop-in load in all of the tested materials except Cu. The reduced pop-in load can be interpreted as the HELP mechanism. Classical dislocation theory was used to model the homogeneous dislocation nucleation and it was shown that H reduces the activation energy for dislocation nucleation. The activation energy for dislocation nucleation is related to the material specific parameters; shear modulus, dislocation core radius and in the case of partial dislocation nucleation, stacking fault energy. These material properties can be influenced by H resulting in a reduced activation energy for dislocation nucleation. The universality of cohesion in metals relates the reduction of the shear modulus to the reduction of the cohesion, meaning HEDE mechanism. The increase in the core radius of a dislocation due to H is a direct evidence of decrease in dislocation line energy and H segregation on the dislocation line. In the case of partial dislocations, the H can segregate on to the stacking fault ribbon and decrease stacking fault energy.

Thus, depending on the experimental approach utilized to probe the H effect, either HELP or HEDE can be observed. In this study by utilizing a proper experimental approach, it was possible to resolve the interconnected nature of the HE.

MM 47.3 Fri 10:55 H 1058

Hydrogen enhanced local plasticity: An atomistic study — •Johann von Pezold and Jörg Neugebauer — Max Planck Institut fuer Eisenforschung, Duesseldorf, Deutschland

The degradation of metals by H-embrittlement is a long-standing problem of huge economic impact, whose underlying mechanisms are still largely unclear, despite extensive research activities. Based on continuum elasticity theory as well as on experimental evidence, various mechanisms for the observed H-induced embrittlement of metals have been proposed, including stress-induced hydride formation, the HELP (hydrogen enhanced local plasticity) and the HEDE (hydrogen enhanced decohesion) mechanisms. However, the atomistic understanding of these mechanisms is still rudimentary.

In this study we consider the atomistic basis for the HELP mechanism, which is based on the assertion that H enhances the mobility of dislocations by shielding the elastic dislocation-dislocation and dislocation-solute interactions. In order to investigate the underlying atomistic mechanisms, the interaction of edge dislocations in Ni with dissolved H atoms has been studied using molecular dynamics simulations in conjunction with the embedded atom method (EAM).

In particular, the stability of isolated H atoms in the stress field of an edge dislocation, as well as the effect of H atoms on the elastic dislocation-dislocation interaction has been considered. In addition, the effect of H atoms on the velocity of an edge dislocation under the influence of an external stress will be presented.

MM 47.4 Fri 11:15 H 1058

Hydrogen-induced plastic deformation of rare earth metal thin films — •Mathias Getzlaff[1] and Astrid Pundt[2] — [1]Inst. of Applied Physics, University of Düsseldorf, D-40225 Düsseldorf — [2]Inst. of Material Physics, University of Göttingen, D-37077 Göttingen

Surface modification of thin Gd films during hydrogen adsorption and absorption has been investigated on the nanometer scale by STM.

The adsorption occurs in two steps. It is initiated by surface imperfections. Starting from these nucleation centers a domain-like spreading is present which is strongly hindered at surface steps.

The measurements have shown that during hydrogen loading two different types of surface pattern develop above a particular concentration: disc-like islands and ramps. These surface patterns can be well described by two plastic deformation processes in the films that lead to glide steps on the film surface: the emission of dislocation loops during hydride precipitation occurs and misfit dislocations near the film-substrate interface. Since plastic deformation leads to stress release we suggest that a lot of thin metal films that are clamped to a substrate relax plastically after reaching a certain hydrogen-induced stress that corresponds to a critical hydrogen concentration. This conclusion is corroborated by the observation that free-standing Gd islands are deformed without structural deformation. Overall, combining the ability of preparing high-quality epitaxial thin films with the detailed analysis of the mechanical properties during hydrogen absorption may lead to a deeper fundamental understanding of hydrogen switchable thin films. It may also improve their industrial applications.

MM 47.5 Fri 11:35 H 1058

Hydrogen interaction with vacancies studied by positron annihilation — •Jakub Cizek — Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Vacancies as open-volume defects provide an additional space in lattice which makes them attractive for hydrogen. Trapping of multiple hydrogen atoms in vacancies was observed in metals. Hydrogen is not only trapped at vacancies existing already in the material, but new vacancies may also be created by hydrogen loading. Positron annihilation spectroscopy (PAS) is a well-developed non-destructive technique with very high sensitivity to open-volume defects, in particular vacancies. Type of defects and defect densities can be determined using PAS. Thus, PAS is an ideal tool for investigations of hydrogen interactions with vacancies. This contribution reports about defect studies of bulk Nb and Pd specimens step-by-step loaded to various hydrogen concentrations. PAS studies were combined with X-ray diffraction and TEM investigations. The experimental data were compared with theoretical calculations of energetic stability and positron characteristics of various defect-hydrogen configurations. We have found that vacancy-hydrogen complexes are introduced into the specimens by hydrogen loading. Density of these vacancy-hydrogen complexes increases with increasing concentration of hydrogen in the specimens. Additional defects are introduced at higher hydrogen concentrations due to precipitation of hydrides. Another type of vacancy-hydrogen complexes can be introduced by electron irradiation. Configuration, stability, and mechanism of formation of the hydrogen-induced defects are discussed.

MM 48: Phase Transitions V

Time: Friday 10:15–11:15 Location: H 0107

MM 48.1 Fri 10:15 H 0107

Adiabatic calorimeter for the determination of thermophysical properties on a metrological basis — •Axel Pramann[1], Hans-Walter Krupke[1], Yosuke Moriya[1,2], Steffen Rudtsch[3], and Stefan Sarge[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Inst. for Solid State Physics, Univ. of Tokyo, 5-1-5 Kashiwanoha, 227-8581 Japan — [3]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

A prototype of a new adiabatic calorimeter in the operation range of 20°C up to 200°C was developed at PTB. The precursor of our calorimeter has been operated at the NBS developed by West and Ginnings [1]. The calorimeter is operated in a step-wise heating mode for the determination of the enthalpy of fusion $\Delta_{\mathrm{fus}}h$, the temperature of fusion and heat capacities of solids. First experiments on Gallium and Indium gave $\Delta_{\mathrm{fus}}h(\mathrm{Ga}) = 80.130 \pm 0.003$ J/g and $\Delta_{\mathrm{fus}}h(\mathrm{In}) = 28.658 \pm 0.003$ J/g. Our experiments confirm the results of Archer and Rudtsch [2, 3] - which can be considered as the currently most accurate reference values - within their given uncertainty. The technical and experimental details as well as the principle of the determination of $\Delta_{\mathrm{fus}}h$ are described on a metrological basis. A further application will be the cryoscopic purity determination of fixed-point materials in thermometry.

[1] E. D. West, D. C. Ginnings, J. Res. Nat. Bur. Stand. 60, 309 (1958).
[2] D. G. Archer, J. Chem. Eng. Data **47**, 304 (2002).
[3] D. G. Archer, S. Rudtsch, J. Chem. Eng. Data **48**, 1157 (2003).

MM 48.2 Fri 10:30 H 0107

Statische atomare Verschiebungen in Cu-reichem Cu-Mn — •Bernd Schönfeld[1], Gernot Kostorz[2], Lee Robertson[3] und Gene Ice[3] — [1]Departement Materialwissenschaft, ETH Zürich — [2]Departement Physik, ETH Zürich — [3]Oak Ridge National Laboratory, USA

Die diffuse Streuung einer einkristallinen Cu-17,2 at.% Mn Probe, die bei 483 K für zwei Wochen ausgelagert worden war, wurde mit Röntgenstrahlen der Energien 6526 eV, 8969 eV und 8909 eV untersucht. Durch die große Variation des Streukontrasts konnten die atomsortenspezifischen statischen Verschiebungen neben den Nahordnungskoeffizienten bestimmt werden. Die beiden eingesetzten Auswertetechniken, die 3λ-Methode und die Georgopoulos-Cohen-Methode, zeigten eine gute Uebereinstimmung in den resultierenden Fourierkoeffizienten. Verschiebungen zwischen nächsten Nachbarn sind dominant und mit 0,0038 nm zwischen Cu-Mn-Paaren am größten. Die Ergebnisse werden mit Resultaten anderer Autoren verglichen und diskutiert.

MM 48.3 Fri 10:45 H 0107

Real-time transmission electron microscopy of equilibrium order fluctuations in Cu_3Au — Xavier Sauvage[1], •Harald Reichert[1], Klaus Mecke[2], Sebastian Kapfer[2], Fritz Phillipp[1], and Helmut Dosch[1,3] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [2]Universität Erlangen-Nürnberg, Staudtstrasse 7, D-91058 Erlangen, Germany — [3]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, Pfaffenwaldring 57, D-70550 Stuttgart, Germany

Using fluctuation microscopy we have monitored local order parameter fluctuations in the binary alloy Cu_3Au in real time with atomic resolution. Close to the phase transformation from the disordered A1 phase to the ordered $L1_2$ structure we found well defined ordered domains with a size of approximately 2nm which are fluctuating on a time scale of 1 second. The morphology of the fluctuations (size and shape) was quantified by Minkowski functionals. The analysis of the Minkowski functionals shows, that although the phase transformation is of first order, the transformation appears to be continuous on a local scale.

MM 48.4 Fri 11:00 H 0107

The influence of elastic strain onto the early stage of decomposition in Cu1,7at.%Fe — •Thomas Rademacher, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Dilute supersaturated Cu Fe alloys have been previously intensely studied in the course of classical homogeneous phase separation neglecting the influence of the anisotropical character of elastic strain.

In a former study HEINRICH et al. (Mat. Sci. Eng. A353 (2003) 92-98) showed that early stages of decomposition at low temperatures of supersaturated Cu Co alloys is mainly controlled by such strain energy. It governs the cluster's size and morphology. It also promotes the formation of chains of precipitates in the elastic soft <100> directions of the Cu-matrix which is in agreement with calculations by MIYASAKI and YAMAUCHI/DE FONTAINE in framework of linear anisotropic elasticity theory. In the current study, these phenomena will be discussed for Cu1,7at%Fe after a heat treatment at 722 K for times ranging from 1,5 to 168 hours. Atom Probe Tomography (APT) was used for measurements as well as the newly developed computer assisted Field Ion Image Tomography (cFIIT) involving an improved reconstruction algorithm which will be presented in short.

Chain like formation of precipitates can be observed. Furthermore the precipitates' positions are systematically determined by computer algorithms and additionally analysed for their relative positions. A preferential alignment in <100> directions can be shown which implies a contribution of the elastic strain on the decomposition behaviour.

MM 49: Phase Transitions VI

Time: Friday 11:45–12:45 Location: H 0107

MM 49.1 Fri 11:45 H 0107

Comparative investigation of nucleation undercooling of Zirconium using the electromagnetic and electrostatic levitation technique — •Stefan Klein[1,2] and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Containerless processing techniques are applied to deeply undercool metallic melts by avoidance of heterogeneous nucleation on container walls. In this work we investigate the nucleation undercooling of Zirconium processed by the electromagnetic and the electrostatic levitation. While in the first case the samples are processed within ultra high purity inert gas atmosphere, the electrostatic levitation allows to process the melts in ultra high vacuum.

We achieved large melt undercoolings of up to 400 K. A statistical analysis of the maximum undercooling observed within a modified model by Skripov gives information about the nucleation mechanism.

The project was funded by Deutsche Forschungsgemeinschaft, under contract No. HE 1601/21.

MM 49.2 Fri 12:00 H 0107

Investigation of the reverted austenite phase in carbon free stainless maraging steel after long term heat treatment — •Stefan Höring, Daniel Abou-Ras, Nelia Wanderka, and John Banhart — Hahn-Meitner-Institut Berlin, Berlin

The main aim of this work was to investigate the microstructure evolution of the carbon free stainless maraging steel Corax after long term heat treatment at 798 K. The mechanical properties of maraging steels are influenced by the amount of reverted austenite. Therefore, the volume fraction, the grain size and the location of the reverted austenite was determined by X-ray diffraction (XRD), scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD). Results of all investigations confirmed that even after long aging time (3000 h) the volume fraction of the austenite is still nearly unchanged. The correlation between crystal orientation of martensite- and the austenite phases is studied by means of EBSD measurements. The austenite grains reached sizes up to 0.05 mm. Long term annealing leads to the formation of new phases located mainly at the grain boundaries. The results of micro-hardness measurements of Corax steel are correlated with the evolution of the microstructure.

MM 49.3 Fri 12:15 H 0107

Formation of Amorphous Domains and Crystalline Precipitates in Precursor Derived Si-C-N-Ceramics — •Wolfgang Gruber and Harald Schmidt — TU Clausthal, Institut für Metallurgie, AG Materialphysik

Precursor derived ceramics of the system Si-C-N are prepared by solid state thermolysis of pre-ceramic polymers at temperatures of about 1100 °C. The materials are free of sinter additives and exhibit a good high-temperature stability and oxidation resistance making them attractive for applications in various branches of technology. Asthermolized ceramics are already separated in silicon rich and carbon rich amorphous phases. Annealing in nitrogen atmosphere at temperatures above the temperature of thermolysis leads to a coarsening of the amorphous phases and at length to the formation of micro crystalline silicon nitride and nano crystalline silicon carbide. According to the phase diagram of the system Si-C-N carbon and silicon nitride are in equilibrium at a nitrogen partial pressure of 1 bar and at temperatures below 1484 °C. At higher temperatures silicon nitride reacts with carbon and silicon carbide and gaseous nitrogen are formed. This reaction and therefore the micro structure of the ceramic strongly depends on temperature and on the nitrogen partial pressure. In this study we investigated the formation kinetics of amorphous domains and crystalline precipitates at different nitrogen partial pressures using small angle X-ray scattering (SAXS) and X-ray diffractometry (XRD).

MM 49.4 Fri 12:30 H 0107

Phase-field simulations of cubic-cubic phase transformations under external load (application to nickel-based superalloys) — •guillaume boussinot[1,2], alphonse finel[1], and yann le bouar[1] — [1]Laboratoire d'Etude des Microstructures, ONERA/CNRS, 92320 Chatillon, France — [2]Institut fur Festkörperforschung, Theorie 3, Forschungszentrum, 52425 Jülich, Germany

In the case of solid-solid transformations involving cubic phases with negative anisotropy (2 C44 > C11 - C12), the three (100)-type directions are equivalent and are the directions perpendicular to which plate-like precipitates minimize the elastic energy (soft directions-Khachaturyan 1983).

When an external uniaxial stress or strain is applied, the equivalence of the (100)-type directions is broken. In superalloys, where an intermetallic phase is dispersed in a disordered matrix, this symmetry breaking leads to an anisotropic coarsening of the microstructure known as rafting. This phenomenon is of great importance in understanding the macroscopic mechanical properties of these systems (via dislocation motion which is almost restricted to the disordered phase).

We will present phase-field simulations of elastically-driven rafting (rafting can be also plastically-driven), requiring the elastic inhomogeneity between the two phases to be taken into account. Different types of rafting are then obtained, which are understood by analyzing the soft directions within an approximation of small inhomogeneity (good for superalloys).

MM 50: Materials Design I

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

MM 50.1 Fri 10:15 H 0111

An adaptive grid algorithm for solving multi-scale solidification processes on large domains — •Sebastian Waniorek, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

To gain insight into interdiffusion microstructures occurring between two contact alloys is critical for the design of new materials and surface coatings. In ternary and more generally multicomponent systems, the so-called Kirkendall effect is accompanied by a phase interface migration, both influencing the material properties. The simulation of interdendritic eutectic growth in one domain is, due to the multiple scales involved, a major challenge in computational engineering. We use a phase-field model coupled with multicomponent diffusion equations to simulate the outlined solidification processes. To numerically solve the phase-field equations with high accuracy, a small physical distance between computation points in the interface is needed. Thus a large computational domain is required to resolve the whole effect. These problems are hardly solvable on a uniform grid due to the vast memory and computation time requirements. However most approaches solve the mentioned equations this way. Since a computation with high resolution is only required in areas of steep gradients, we adapt the computation grid to the accuracy affordances. By this approach, the computation effort in the bulk solid phase and in liquid regions is minimized. We apply the method of adaptive mesh refinement to a finite difference solver and enable computations of multicomponent diffusion processes even on personal computers.

MM 50.2 Fri 10:30 H 0111

Post-Machining Thermal Treatment after Surface Finishing of Hardened Steels: Kinetics of XRD Line Width Reduction and Improvement in Rolling Contact Lifetime under Mixed Friction Conditions — •Jürgen Gegner — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Hard surface finishing represents the final manufacturing step for functional areas of machine elements in state-of-the-art production. Raceways of rolling bearing rings are ground and honed to the required low roughness. Plastic deformation is restricted to a narrow edge zone of the hardened steel. Reheating of the machined components below the martensite tempering or bainite transformation temperature results in a marked decrease of the XRD line width on the surface. The investigated samples are made of through-hardened standard bearing steel 100Cr6 (international denotation: SAE 52100). On the basis of a material model that explains the effect as a complex diffusion process of dislocational carbon segregation, i.e. static strain aging, the measured kinetics of the XRD line width reduction is simulated by an Arrhenius-type equation, which describes the rate-controlling reaction step of temper carbide dissolution. The formation of a small white-etching surface layer of around 1 um thickness by post-machining thermal treatment (PMTT) strongly supports this assumption. First rig tests suggest a considerable increase of the lifetime of Hertzian loaded elements that operate under heavy surface loading. PMTT performed in air leads to a beneficial nanoscaled oxide layer.

MM 50.3 Fri 10:45 H 0111

Long-life Bismuth Liquid Metal Ion Source for Micromachining Application. — •Paul Mazarov, Alexander Melnikov, Rolf Wernhardt, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum 44780, Germany

Liquid metal ion sources (LMIS) are widely used in focused ion beam (FIB) technology for micromachining and surface treatment, and thus LMIS have been broadly developed. Key features of a LMIS for 3D-microfabrication of materials are long life-time, high brightness, stable ion current and a highly effective milling ability for the material to be modified. The most widely used LMIS with such properties is the Ga LMIS, being the working horse of FIB today. A very successful approach to increase the material removal rate, according to sputter theory, is the use of heavier ions and their clusters. We have produced a new long-life (about 1000 h) Bi LMIS with a good beam performance. The investigation of the sputtering rate of NiTi shape memory alloys using Ga and Bi LMIS shows that, for the same experimental conditions, the material removal rate with using of Bi ions without a mass separator is about 5 times larger compared to Ga ions. The sputter threshold dose is nearly one magnitude lower than that of Ga. For many applications this means a drastical reduction of working time. This sputter enhancement is particularly pronounced for target materials with large atomic masses. Furthermore, the roughness induced by the cluster projectile impact is much less pronounced than that generated by the atomic projectiles and the penetration depth is smaller, leading to less contamination of the target.

MM 50.4 Fri 11:00 H 0111

SRμCT in Materials Science at the Beamline HARWI II — •Julia Herzen, Felix Beckmann, Astrid Haibel, Tilman Donath, Funda S. Bayraktar, Stefan Riekehr, Mustafa Kocak, and Andreas Schreyer — GKSS Research Centre, Max-Planck-Str.1, 21502 Geesthacht

The synchrotron radiation based micro tomography is a powerful imaging tool in the wide range of materials science. Compared to laboratory X-ray sources the micro tomography at a synchrotron allows to visualize non-destructively high and low absorbing materials without any beam hardening effect and with a very high density resolution.

The beamline HARWI II operated by the GKSS Research Centre in cooperation with Deutsches Elektronen-Synchrotron DESY, Hamburg is designed for materials science experiments using hard X-rays. A fixed-exit monochromator provides a highly intense, monochromatic X-ray beam in the energy range between 15 and 200 keV. This large range of photon energies, the spatial resolution down to 3 μm and the high density resolution are important for microtomographic applications. The advantages of the beamline are demonstrated for absorption contrast tomography study of crack propagation within laser welded Al-Alloy T-Joints.

MM 51: Materials Design II

Time: Friday 11:45–13:00 Location: H 0111

MM 51.1 Fri 11:45 H 0111

High strength conductors: CuAg tapes — •Jens Freudenberger, Julia Lyubimova, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials; PO-Box 270116; D-01171 Dresden

Conductor materials with a high mechanical strength and a high electrical conductivity are required for a number of applications. There especially is a growing interest in tapes and strips for connectors. CuAg tapes, prepared by conventional casting, heat treatment and rolling, show the beneficial combination of high electrical conductivity and high mechanical strength. A combination of 60%IACS and 1.2GPa is achieved and referred to the microstructure of the material.

MM 51.2 Fri 12:00 H 0111

Formation of complex 3D networks of anisotropic colloidal nanocrystals — •Stefan Kudera[1], Isabella Franchini[2], Joachim P. Spatz[1], and Liberato Manna[2] — [1]Max Planck Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]National Nanotechnology Laboratories of CNR-INFM, Via Arnesano, 73100 Lecce, Italy

Semiconductor nanocrystals can be synthesised in a variety of different shapes. There are standard procedures for the production of spheres and anisotropic nanorods. Additionally it is possible to introduce branching points into the structures in order to obtain objects of a more complicated shape such as bumerang shaped dipods or tetrapods.

Here, we will present a possibility to interconnect colloidal nanocrystals into complex networks. These networks are formed in a solution and they are stable for a certain amount of time, during which they might be deposited on any kind of substrate. Generally the time available for the treatment of the networks is of the order of few minutes. A metallic domain acts as linker between the individual nanocrystals.

As the networks are formed of semiconductor materials they are of interest for the production of solar cells. When embedded into a hole transporting polymer, the nanocrystal network might enable an efficient electron transport towards the anode. Thus, while providing a good electronic contact with the electrode, the network still offers a large surface, on which the charges could be separated.

MM 51.3 Fri 12:15 H 0111

Probing the rattling mode scenario in nano-cage based thermoelectric materials — Andreas Leithe-Jasper[1], Yuri Grin[1], Walter Schnelle[1], Romain Viennois[1], Hannu Mutka[2], Lucia Capogna[2], Mark Robert Johnson[2], and •Michael Marek Koza[1,2] — [1]MPI-CPfS, Noethnitzer Strasse 40, D-01187 Dresden — [2]ILL, 6 Rue Jules Horowitz, F-38042 Grenoble

The direct conversion of waste heat into electrical power in thermoelectric devices is believed to contribute substantially to future power supply and sustainable energy management. Nanocage-based crystalline structures like filled skutterudite systems XFe4Sb12 (X = Ca, Cs, Ba, La, Ce, Yb, Nd, ...) and clathrate materials like BaGe and BaSi have attracted some scientific interest as they are sought to be excellent thermoelectric materials. Their applicability for an efficient conversion of thermal into electrical energy is based on the opportunity of tuning appreciably the heat transport through the sample leaving the electron transport rather unaffected.

We will give some examples of our experimental work comprising neutron scattering techniques and bulk spectroscopies, e.g. specific heat measurements, on filled skutterudite systems and pyrochlore osmates XOs2O6 (X = K, Rb, Cs). We will present a new approach based on ab initio lattice dynamics calculations towards the interpretation of experimental data particularly dedicated to polycrystalline systems. We will show that the apparently established picture of rattling modes, i.e. decoupled dynamics of guests X and host Fe4Sb12 is not correct.

MM 51.4 Fri 12:30 H 0111

Ab initio up to the melting point: Influence of vacancies and explicit anharmonicity — •Blazej Grabowski, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Str. 1, 40237 Düsseldorf, Deutschland

A recent study [1] on an extensive set of elementary metals showed that a wide variety of thermodynamic properties can be excellently reproduced within the quasiharmonic approximation. An exception is the heat capacity which shows a clear deviation from experiment at temperatures above 70% of the melting temperature.

To clarify the origin of the nonlinear increase, we have investigated two potential candidate mechanisms being debated controversially in the literature. On the one hand, we have calculated the contribution of monovacancies to the free energy. We have included the vibrational entropy of the vacancy using the full volume dependent dynamical matrix (quasiharmonic approximation). On the other hand, we have calculated the contribution of the volume dependent explicit anharmonicity (of the pure crystal) to the free energy. For this purpose, we have employed thermodynamic integration. We find that both contributions are of equal magnitude and correct the quasiharmonic results when compared to experiment.

[1] Grabowski B., Hickel T., and Neugebauer J., PRB 76, 024309 (2007).

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Scalable molecular dynamics simulations of oxides — •Peter Brommer and Franz Gähler — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

Due to polarisable oxygen atoms and long-range ionic interactions, molecular dynamics (MD) simulations of oxides usually scale unfavourably with the system size. By using the direct summation technique described by Wolf *et al.* [1] with a slightly increased interaction cut-off radius, contributions in reciprocal space can be neglected, and the simulation scales linearly with the system size. Additionally, direct summation methods can be used within the framework of an existing MD programme, including parallelisation algorithms and freedom in the choice of boundary conditions. We present an implementation of the silica interaction potential of Tangney and Scandolo [2] using Wolf summation. This model treats the oxide atoms as polarisable, and the dipole strengths are determined in a self-consistency loop. We demonstrate the scaling properties and discuss the validity of using Wolf summation for this potential.

[1] Wolf *et. al*, J. Chem. Phys. **110**, 8254 (1999)
[2] Tangney and Scandolo, J. Chem. Phys. **117**, 8898 (2002)