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

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Overview of Invited Talks and Sessions

(lecture rooms H16, H4, and H6; Poster C)

Invited Talks

MM 1.1	Mon	9:30–10:00	H16	**Size Effects in Metal Plasticity** — •Erica Lilleodden
MM 2.1	Mon	10:15–10:45	H16	**Effect of hydrogen and grain boundaries on dislocation nucleation and multiplication examined with a Ni-AFM** — •Horst Vehoff, Afrooz Barnoush
MM 7.1	Mon	14:00–14:30	H16	**Metallic Glasses** — •Lindsay Greer
MM 13.1	Tue	9:30–10:00	H16	**Computational Materials** — •Sidney Yip
MM 14.1	Tue	10:15–10:45	H16	**Micromechanics inside the SEM** — •Benedikt Moser
MM 19.1	Tue	14:00–14:30	H16	**Development of Platinum-Based Superalloys by Optimization of Microstructure** — •Uwe Glatzel
MM 21.1	Wed	14:00–14:30	H16	**XRD residual stress analysis: one of the few advanced physical measuring techniques that have established themselves for routine application in industry** — •Wolfgang Nierlich, Jürgen Gegner
MM 27.1	Thu	9:30–10:00	H16	**Atomic Migration Phenomena in Intermetallics with High Superstructure Stability** — •Rafal Kozubski, Véronique Pierron-Bohnes, Wolfgang Pfeiler
MM 34.1	Thu	14:00–14:30	H16	**Shape-Memory Polymers** — •Andreas Lendlein
MM 40.1	Fri	10:15–10:45	H16	**Material science with positrons: From Doppler-Spectroscopy to Failure Prediction** — •Matz Haaks

Sessions

MM 1.1–1.1	Mon	9:30–10:00	H16	**HV Lilleodden**
MM 2.1–2.5	Mon	10:15–12:15	H16	**SYM Micro- and Nanomechanics I**
MM 3.1–3.4	Mon	10:15–11:15	H4	**Liquid and amorphous materials I**
MM 4.1–4.5	Mon	11:45–13:00	H4	**Liquid and amorphous materials II**
MM 5.1–5.4	Mon	10:15–11:15	H6	**Interfaces I**
MM 6.1–6.5	Mon	11:45–13:00	H6	**Interfaces II**
MM 7.1–7.1	Mon	14:00–14:30	H16	**HV Greer**
MM 8.1–8.6	Mon	14:45–17:00	H16	**SYM Micro- and Nanomechanics II**
MM 9.1–9.4	Mon	14:45–15:45	H4	**Liquid and amorphous materials III**
MM 10.1–10.5	Mon	16:15–17:30	H4	**Liquid and amorphous materials IV**
MM 11.1–11.4	Mon	14:45–15:45	H6	**Interfaces III**
MM 12.1–12.6	Mon	16:15–17:45	H6	**Growth**
MM 13.1–13.1	Tue	9:30–10:00	H16	**HV Yip**
MM 14.1–14.6	Tue	10:15–12:15	H16	**SYM Micro- and Nanomechanics II**
MM 15.1–15.4	Tue	10:15–11:15	H4	**Phase transitions I**
MM 16.1–16.4	Tue	11:45–12:45	H4	**Phase transitions II**
MM 17.1–17.4	Tue	10:15–11:15	H6	**Hydrogen in materials**
MM 18.1–18.4	Tue	11:45–12:45	H6	**Electronic properties I**
MM 19.1–19.1	Tue	14:00–14:30	H16	**HV Glatzel**

MM 20.1–20.55	Tue	14:45–18:00	Poster C	**Poster session**
MM 21.1–21.1	Wed	14:00–14:30	H16	**HV Nierlich**
MM 22.1–22.14	Wed	14:45–19:55	H16	**SYM Physics meets Industry**
MM 23.1–23.6	Wed	14:45–16:15	H4	**Nano structured materials I**
MM 24.1–24.6	Wed	16:45–18:15	H4	**Nano structured materials II**
MM 25.1–25.6	Wed	14:45–16:15	H6	**Electronic properties II**
MM 26.1–26.6	Wed	16:45–18:15	H6	**Electronic properties III**
MM 27.1–27.1	Thu	9:30–10:00	H16	**HV Kozubski**
MM 28.1–28.4	Thu	10:15–11:15	H16	**Intermetallic phases I**
MM 29.1–29.5	Thu	11:45–13:00	H16	**Intermetallic phases II**
MM 30.1–30.4	Thu	10:15–11:15	H4	**Phase transitions III**
MM 31.1–31.4	Thu	11:45–12:45	H4	**Nano structured materials III**
MM 32.1–32.4	Thu	10:15–11:15	H6	**Diffusion and point defects I**
MM 33.1–33.4	Thu	11:45–12:45	H6	**Diffusion and point defects II**
MM 34.1–34.1	Thu	14:00–14:30	H16	**HV Lendlein**
MM 35.1–35.28	Thu	14:45–20:45	H16	**SYBM Bioinspired Materials**
MM 36.1–36.6	Thu	14:45–16:15	H4	**Nano structured materials IV**
MM 37.1–37.5	Thu	16:45–18:00	H4	**Nano structured materials V**
MM 38.1–38.4	Thu	14:45–15:45	H6	**Diffusion and point defects III**
MM 39.1–39.8	Thu	16:15–18:15	H6	**Mechanical properties I**
MM 40.1–40.1	Fri	10:15–10:45	H16	**HV Haaks**
MM 41.1–41.4	Fri	11:00–12:00	H16	**Materials design I**
MM 42.1–42.4	Fri	12:30–13:30	H16	**Materials design II**
MM 43.1–43.4	Fri	11:00–12:00	H6	**Mechanical properties II**
MM 44.1–44.4	Fri	12:30–13:30	H6	**Mechanical properties III**

Symposium Bio-inspired Materials (SYBM)
offered jointly by the sections of MM (Metal and Material Physics), BP (Biological Physics), CPP (Chemical and Polymer Physics), DS (Thin Layers) and DY (Dynamics and Statistical Physics). Thursday, March 29, one-day-symposium, continuation 14:45 H16 and poster session starting 19:00 (MM35).

Organizers:
Prof. Dr. Eduard Arzt
Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart
Prof. Dr. Peter Fratzl
Department für Biomaterialien, MPI für Kolloid - und Grenzflächenforschung, D-14476 Potsdam
PD Dr. Peter Müller-Buschbaum
Physik-Department E13, Technische Universiät München, D-85747 Garching

Nature provides a wide source of inspiration for chemists, physicists and engineers to create highly sophisticated functional materials. Many natural materials with complex, often hierarchical structure provide an unequalled level of adaptivity, multifunctionality, and mechanical performance. Biomimetic materials research provides a unique opportunity for physicists in a rapidly expanding field between the worlds of biology, physics and materials science. It starts by elucidating the physical origins of the outstanding functionality of biological materials, and aims at designing improved or even radically new materials based on the knowledge of natural systems. Bioinspired materials will have an impact on various fields, from engineering to functional materials, as well as regenerative medicine.

Symposium Strain Engineering for New Functional Structures (SYSE)
jointly proposed by the sections of DF(Dielectric Solids), HL (Semiconductors), DS (Thin Layers) and MM (Metal and Material Physics).

Symposium Physics meets Industry (MM 22)
Physical Measuring Techniques for Industrial Requirements Besides the description of open measuring problems in the field of materials physics and techniques this forum promoting the exchange

of information between physicists and engineers from industry, universities and research institutes is focusing on new physical measuring techniques and their commercialisation as well as on recent success stories.
Organizers:
Dr. Jürgen Gegner
SKF GmbH, Werkstoffphysik - STW3, Ernst-Sachs-Str. 5, D-97424 Schweinfurt
Prof. Dr. Ferdinand Haider
Institut für Physik, Lehrstuhl Exp. Physik 1, Universität Augsburg, Universitätsstr. 1, D-86135 Augsburg

Symposium Micro- and Nanomechanics (MM 2, MM 8, MM 14)
An insight into the micro- and nanomechanical properties of materials and structures is becoming more and more important in the development of new advanced materials and small devices. New microtesting techniques such as nanoindentation, nanopillar testing and microtensile tests allow us to study these properties on a very small scale. They are especially suitable for investigating features of nanostructured materials and thin films, and for evaluating the size effects which influence mechanical behaviour on the nanoscale. This symposium will present recent progress in the field of nanomechanical testing in several talks by leading experts in this field.
Organizers:
Prof. Dr. Mathias Göken
Institut für Werkstoffwissenschaften I, Universität Erlangen-Nürnberg, Martensstraße 5, 91058 Erlangen
Prof. Dr. Jörg Löffler
Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Wolfgang-Pauli-Str. 10, CH-8092 Zürich

Symposium Magnetic Shape Memory Alloys,
organized together with the sections of MA (Magnetism) and DS (Thin Layers)
The new class of magnetic shape memory (MSM) alloys allows the modification of structure and microstructure of solid materials by external magnetic fields. Since their discovery in 1996, the strain obtained in these smart materials has significantly increased and can reach up to 10%. This makes these materials very interesting for actuator and sensor applications and motivates the examination of the underlying microscopic mechanism and the search for new and better materials. The MSM effect originates from the interaction of magnetism and microstructure. As the application of MSM alloys in microsystems is very promising, a lot of research is conducted on thin films. Thus a joint symposium of MA, MM and DS is appropriate for this interdisciplinary topic. The DFG recently started to support this area within the priority program SPP 1239 'Modification of microstructure and shape of solid materials by external fields', which is coordinated by Dr. S. Fähler (http://www.magneticShape.de).

For the program see MA.

Annual General Meeting of the Section Metal and Material Physics

Tuesday 18:00–19:00 H33

- Report of the chairman of the section Metal and Material Physics
- Election of the chairman of the section Metal and Material Physics.
- Invited talks and symposia for the next spring meeting 2008 in Berlin.
- Other topics

MM 1: HV Lilleodden

Time: Monday 9:30–10:00 Location: H16

Invited Talk MM 1.1 Mon 9:30 H16

Size Effects in Metal Plasticity — •Erica Lilleodden — GKSS Forschungszentrum, Institut für Werkstoffforschung, Max-Planck-Straße 1, D-21502 Geesthacht

Size effects in plasticity have received much attention in recent years, due to increased resolution in experimental capabilities, and the development of materials at small geometric and microstructural length scales. Nanoindentation, wafer curvature and, more recently, micro-compression tests have all shown such size effects. To date, a multitude of theories for the observed behaviors exist based on the evolution of dislocation distributions, and are often conflicting. This talk will provide an overview of recent experimental studies of size effects in materials, particularly those which combine nanoindentation-based techniques with microstructural characterizations (e.g., transmission electron microscopy, orientation imaging microscopy and x-ray microdiffraction). The overwhelming observation of "smaller is stronger" will be discussed in terms of the volume of deformation, the presence of strain gradients, and the evolution of dislocation structure.

MM 2: SYM Micro- and Nanomechanics I

Time: Monday 10:15–12:15 Location: H16

Invited Talk MM 2.1 Mon 10:15 H16

Effect of hydrogen and grain boundaries on dislocation nucleation and multiplication examined with a Ni-AFM — •Horst Vehoff and Afrooz Barnoush — Institut für Werkstoffwissenschaft, Universität des Saarlandes, 66041 Saarbrücken

A nanoindenting AFM with an environment chamber was constructed to study the effect of hydrogen on decohesion and dislocation nucleation and the effect of grain boundaries on dislocation nucleation. Ultra fine grained Ni and Ni single crystals were examined. It could be clearly shown that hydrogen influences the pop in width and length. Testing single grains with grain sizes below one micron at different rates inside a Ni-AFM showed that the rate dependence of UFG Ni is a result of the interaction of the growing dislocation loop with the boundary. The results will be discussed in the talk.

MM 2.2 Mon 10:45 H16

Size effects observed during indentation testing — •Karsten Durst — Institut für Werkstoffwissenschaften 1, Universität Erlangen-Nürnberg, Erlangen

Nanoindentation allows probing the mechanical response of materials from the nanoscale to the macroscale. It is found that strength of crystalline materials is size dependent and the size dependence is influenced by i.e. grain size, dislocation density and solid solution strengthening. Initially, materials deform purely elastically, supporting loads up to their theoretical strength. The nucleation and multiplication of dislocations leads to a discontinuity in the load displacement data, marking the transition from elastic to plastic deformation. After pop-in, a high hardness is observed, which decreases with increasing indentation depth until a constant hardness is found for large indentation depths. The experimental observations can be modeled within the framework of Taylor hardening, considering geometrically necessary dislocations (GND) and statistically stored dislocations (SSD). The statistically stored dislocation density is derived from uniaxial stress-strain data applying the Tabor concept of the representative strain. The GNDs are necessary for providing the lattice rotation underneath the indenter and for forming the residual impression. Their density is calculated for conical and spherical indenters, using the storage volume of GNDs as a fitting factor for describing the experimental observations. Hertzian contact theory is used to describe the initial elastic deformation of the material, whereas the critical pop-in load is derived from the theoretical strength of the material.

MM 2.3 Mon 11:15 H16

Micro-Compression Testing of Metals — •Cynthia Volkert — Institut für Materialforschung II, Forschungszentrum Karlsruhe, 76021 Karsruhe, Germany

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. The opportunity to tailor mechanical properties by changing the material length scale, and to combine this with desired electrical, magnetic or chemical properties, has been a major incentive for the development of nanostructured metals and composites for technological applications.

Recent developments in micro-mechanical testing methods using focused ion beam machining offer unique opportunities to systematically study deformation of small samples. This talk will focus on results from uniaxial compression tests on sub-micron columns of single crystal Au and nanoporous Au. The experiments confirm that *smaller is stronger*, with sub-micron specimen strengths close to theoretical values. In addition to high strength, the nanoporous Au exhibits macroscopic brittle behavior. Results from fracture testing of micron-sized, notched cantilever beams fabricated in nanoporous Au with a focused ion beam reveal that the material has mechanical properties similar to those of a porous ceramic. These trends will be discussed in terms of the inhibition of defect creation and motion in small volumes. Finally, an outlook of what can be achieved by tailoring length scales in various materials will be presented.

MM 2.4 Mon 11:45 H16

Of Pillars and Bridges, Mechanical Testing of Micro and Nano Structures — •Holger Pfaff[1] and Erik Herbert[2] — [1]Surface, Rheinstrasse 7, 41836 Hückelhoven — [2]MTS Nano Instruments, 1001 Larson Drive, Oak Ridge, TN 37830

Successive miniaturization in technology and science has created a strong need for testing materials and structures in the nano scale. As microscopic structures and thin coatings often behave significantly different from bulk materials, a detailed understanding of the underlying mechanisms is crucial for the fabrication of reliable micro products and for further technological and scientific progress.

Surface detection, accurate displacement and load control, as well as precise lateral positioning are critical issues for investigating the mechanical behavior of micro and nano structures. Hence insensitive surface detection would damage the specimen before the test. By measuring the dynamic contact stiffness, the sensitivity of surface detection is increased significantly.

The requirements of locating and addressing submicron scale features on a surface are met by scanning the specimen with the very probe used for the mechanical testing.

Several methods, combining the mentioned techniques, were developed for automatically testing fragile structures in a complex sequence of testing steps. The methods were used for investigating the mechanics of MEMS devices and fibrillar polymer structures.

MM 2.5 Mon 12:00 H16

Investigation of the size dependent plasticity of micro-pillars by discrete dislocation dynamics — •Daniel Weygand[1], Jochen Senger[1], Oliver Kraft[1,2], and Peter Gumbsch[1,3] — [1]IZBS, University of Karlsruhe, Karlsruhe, Germany — [2]IMF II, Forschungszentrum Karlsruhe, Germany — [3]IWM, Fraunhofer Institut, Freiburg, Germany

The understanding of the plasticity of sub-micrometer sized metallic components is of relevance due to the increasing use of small scale devices. The reliability of such structures is of importance for technical applications. As indicated by many experimental studies on sub-micron sized samples, crystalline materials in general display pronounced size effects regarding their mechanical behavior. In order to investigate the microstructural origin of the size effect the plastic flow of uniformly loaded pillars is modelled using a three dimensional discrete dislocation dynamics tool. Starting from Frank-Read sources of

given length and random orientation, the simulated flow stress at 0.2% plastic strain shows a size effect, quite similar to experimental findings for larger strains. Furthermore the scattering in the simulated stress-strain curves decreases with increasing sample size, which reflects that plasticity of small scale samples is very sensitive to the underlying dislocation microstructure. Statistical properties of the resulting dislocation microstructure are discussed as well.

MM 3: Liquid and amorphous materials I

Time: Monday 10:15–11:15 Location: H4

MM 3.1 Mon 10:15 H4

Neutron scattering investigatons on melts of Al-Ni and Zr-Ni alloys — •Dirk Holland-Moritz[1], Andreas Meyer[1], Helena Hartmann[1], Sebastian Stüber[2], and Fan Yang[2] — [1]Institut für Materialphysik im Weltraum, DLR-Köln, Germany — [2]Physik Department E13, TU-München, Germany

This work presents investigations on the short-range order of stable and deeply undercooled melts of binary Al-Ni and Zr-Ni alloys. The liquids were containerlessly processed and undercooled by use of the electromagnetic levitation technique which was combined with the technique of elastic neutron scattering at the diffractometer D20 of the Institut Laue-Langevin (ILL) in order to determine the static structure factor. The scattering contrast was varied by isotopic substitution. By means of this partial structure factors were determined. For the case of $Zr_{64}Ni_{36}$ alloys strong indications for the existence of a chemical order are found.

This work was supported by DFG under contracts No. Ho1942/6-3 and Me1958/2-3.

MM 3.2 Mon 10:30 H4

Interplay of Structure and Dynamics in liquid and undercooled AlNi melts — •Sebastian Stüber[1], Andreas Meyer[2], Dirk Holland-Moritz[2], Helena Hartmann[2], and Tobias Unruh[3] — [1]Physik Department E13, TU München — [2]Institut für Materialphysik im Weltraum, DLR Köln — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching

AlNi melts show a chemical short-range order (CSRO), dependent on the Ni concentration [1]. For lower temperatures, this CSRO becomes more pronounced. To increase the available temperature range further, we used electromagnetic levitation. This container-free method enabled significant undercooling (up to 266 K) for several hours.

The AlNi melts were studied using inelastic neutron scattering. The quasielastic line was fitted by a scaled Lorentzian, whose HWHM corresponds to the inverse of the mean relaxation time τ_q. With this a q-dependent diffusivity $D(q) = 1/(\tau q^2)$ can be defined, for the hydrodynamic limit $q \to 0$ one gets the (Ni) self-diffusion coefficient D as a function of temperature.

The q-dependent diffusivity $D(q)$ provides information about the correlation between the diffusive motion and the CSRO, visible at intermediate q values. Using $D(q)$ we will discuss the process of diffusive atomic motion in AlNi melts, under the pronounced influence of CSRO.

[1] S.K. Das *et al.*, Appl. Phys. Lett. **86**, 011918 (2005).

MM 3.3 Mon 10:45 H4

Struktur und Dynamik von flüssigem Titan: Computersimulation, Modenkopplungstheorie und Experiment — •Jürgen Horbach — Institut für Physik, Universität Mainz, Staudinger Weg, D-55099 Mainz

Mittels Molekulardynamik-Computersimulationen wird die Struktur und Dynamik von Titan in der Nähe des Schmelzpunktes, d.h. bei der Temperatur $T = 1970\,\mathrm{K}$, untersucht. Dabei verwenden wir als Modell ein Potential vom "embedded atom"-Typ [1]. Der statische Strukturfaktor $S(q)$ aus der Simulation ist in sehr guter Übereinstimmung mit experimentellen Daten [2,3]. Wir verwenden den simulierten Strukturfaktor $S(q)$ als Input für eine Rechnung im Rahmen einer Modenkopplungstheorie, aus der die von der Frequenz ω abhängigen, dynamischen Strukturfaktoren $S(q,\omega)$ vorhergesagt werden. Wir zeigen, dass die dynamischen Strukturfaktoren aus der Theorie in semiquantitativer Übereinstimmung mit der Simulation sind.

[1] R. Zope, Y. Mishin, Phys. Rev. B **68**, 024102 (2003).

[2] G. W. Lee, A. K. Gangopadhyay, K. F. Kelton, R. W. Hyers, T. J. Rathz, J. R. Rogers, D. S. Robinson, Phys. Rev. Lett. **93**, 037802 (2004).

[3] D. Holland-Moritz, O. Heinen, R. Bellissent, Th. Schenk, Mat. Sc. Eng. A, in press (2006).

MM 3.4 Mon 11:00 H4

Thermophysical properties of Si, Ge and Si-Ge melts under microgravity — •Suresh Mavila Chathoth, Bernd Damaschke, and Konrad Samwer — I. Physikalisches Institut, Universitaet Göttingen, 37077 Göttingen, Germany

The liquid Si and Ge are highly reactive materials. Especially the liquid Si is known to reactive with almost all materials. To have an accurate values of thermophysical properties of these melts container less processing is required. The container less processing can be realized by electromagnetic or electrostatic levitation. These ground based levitation techniques have demerits of gravity driven convection and accuracy of the data depend on convection currents. The thermophysical properties of Si, Ge and Si-Ge alloy melts have been investigated in the TEMPUS facility on board of Zero-G plane during the parabolic flights. Unlike metallic alloys [1] which can melt in a magnetic field, Si, Ge and Si-Ge are semiconductors in their sold state a laser pre-heating was necessary to melt these samples. The melted droplets were video taped and from the images the thermal expansion and surface tension of the samples were evaluated. Absence of gravity driven convection a separation of the influence of gravity induced convection become possible by comparing the data with ground based experiments. The work was supported by BMBF/DLR under grant No. 50WM0541.

[1] B. Damaschke, D. Oelgeschlaeger, J. Ehrich, E. Dietzsch, and K. Samwer, Rev. Sci. Instrum. **69**, 2110 (1998).

MM 4: Liquid and amorphous materials II

Time: Monday 11:45–13:00 Location: H4

MM 4.1 Mon 11:45 H4

Devitrification, consolidation and mechanical properties of ball milled Al-Y-Ni-Co glassy ribbons — •Kumar Babu Surreddi[1], Sascha Sager[2], Mira Sakaliyska[1], Sergio Scudino[1], and Jürgen Eckert[1] — [1]IFW Dresden, Institut für Komplexe Materialien, Postfach 27 01 16, D-01171 Dresden, Germany — [2]FG Physikalische Metallkunde, FB 11 Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstraße 23, D-64287 Darmstadt, Germany

In this work, glassy powders have been obtained by ball milling of Al-Y-Ni-Co glassy ribbons. The pulverization of the melt-spun ribbons was achieved by using proper milling conditions, i.e. interval-milling at low intensity, corresponding to a rather low kinetic energy, and performed at cryogenic temperature in order to retain their glassy structure and to avoid sticking of the material to the milling tools due to the high ductility of the ribbons. Due to the controlled milling conditions, the ball milled ribbons display a strikingly similar structure and crystallization behavior compared to the parent as-spun sample. The crystallization behavior and the temperature dependence of the viscosity of the as-spun and the milled ribbons were studied in order to select the proper consolidation parameters. Fully glassy and glassy-Al composite powders were then consolidated through uniaxial hot pressing and hot extrusion and finally the mechanical properties of the bulk specimens were evaluated via room temperature compression tests.

MM 4.2 Mon 12:00 H4

Crystallization behavior and consolidation of ball milled Zr60Ti5Ag5Cu12.5Ni10Al7.5 glassy powders — •Sergio Scudino, Shankar Venkataraman, Mira Sakaliyska, Kumar Babu Surreddi, and Jürgen Eckert — IFW Dresden, Institut für Komplexe Materialien, Postfach 27 01 16, D-01171 Dresden, Germany

Devitrification and consolidation of Zr60Ti5Ag5Cu12.5Ni10Al7.5 glassy powders produced by ball milling of intermetallic compounds have been investigated. The crystallization behavior is characterized by the formation of a nanoscale quasicrystalline phase along with a minor amount of tetragonal Zr2Cu phase during the first stage of the crystallization process. In the second crystallization event the metastable QC transform into the tetragonal Zr2Cu phase. The viscous flow of the supercooled liquid was studied by parallel plate rheometry, showing a distinct viscosity drop related to the glass transition, corroborating the results from DSC measurements. Consolidation of the glassy powders was performed by uniaxial hot pressing. The consolidation parameters were properly selected in order to obtain partially crystallized bulk samples with a composite microstructure characterized by the contemporary presence of glassy, quasicrystalline and tetragonal Zr2Cu phases. Hardness measurements reveal a Vickers hardness of 4.61 GPa and an estimated yield strength of 1.53 GPa. These results show that powder metallurgy methods are suitable for the production of Zr-based alloys characterized by a composite microstructure consisting of glassy, quasicrystalline and crystalline phases with mechanical properties similar to materials prepared by other techniques.

MM 4.3 Mon 12:15 H4

Metallurgical considerations in the development of ferromagnetic Fe-based metallic glasses — •Giovanni Mastrogiacomo and Jörg Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Wolfgang-Pauli-Str. 10, 8093 Zurich, Switzerland

Despite intense research activity concerning the glass-forming ability of metallic alloys, the crucial metallurgical parameters for improving glass-forming ability are still not well understood. Considering the crystallization of several bulk metallic glasses which decompose in the deeply undercooled liquid region, we developed Fe-based bulk metallic glasses by a further destabilization of the Fe–Cr–Co system. This system tends to decompose in iron-rich and chromium-rich b.c.c. phases [1]. The liquidus temperature was systematically reduced by alloying elements which satisfy the empirical rules suggested by Hume-Rothery and destabilize the high temperature austenitic phase. The resulting metallic glasses of composition $(Fe_{0.582}Co_{0.418})_{80}Cr_{10}Zr_{10}$ and $[(Fe_{0.582}Co_{0.418})_{0.81}Cr_{0.1}Zr_{0.07}Ti_{0.02}]_{90}B_{10}$ reveal unexpected magnetic properties, as, for example, inverted major and exchange-biased minor hysteresis loops [2,3]. These results are discussed considering the decomposing tendency of the Fe–Cr–Co system.

[1] F. Zhu, P. Haasen, and R. Wagner, Acta Metall. **34**, 457 (1986).
[2] G. Mastrogiacomo *et al.*, J. Appl. Phys. **99**, 023908 (2006).
[3] G. Mastrogiacomo *et al.*, J. Appl. Phys. **100**, 12xxxx (2006).

MM 4.4 Mon 12:30 H4

Self-assembly of monatomic complex crystals and quasicrystals with a double-well potential — •Michael Engel and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

For the study of crystal growth and dynamics a simple two-dimensional monatomic model system with three parameters is introduced. Depending on the value of the parameters several complex crystals, a decagonal quasicrystal, and a dodecagonal quasicrystal are stabilized in thermal equilibirum. They show up in the phase diagram of the system, which we calculate using molecular dynamics simulations. The observed crystals can have unit cells larger than the interaction radius. When growing the complex (quasi-)crystals from the liquid state, a continuous amelioration of the structure by diffusion processes is observed. This is accomplished by discrete atomic jumps over well-defined jump distances. For the investigation an interactive virtual lab is used, that allows a direct observation and control of the simulation dynamics.

MM 4.5 Mon 12:45 H4

Phason flips and solitons in the dynamic Fibonacci chain — •Hansjörg Lipp, Steffen Sonntag, Michael Engel, and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Quasicrystals possess the phason degree of freedom which manifests itself in correlated atomic flip motions. To get insight into the microscopic dynamics of the flips, we studied one dimensional model systems: periodic and quasiperiodic anharmonic chains, in particular the quasiperiodic Fibonacci chain.

Here we present approximate analytic solutions of the equations of motion in such systems as well as results from molecular dynamics simulations. The chains show localized modes interacting with phonons. There are both breathers and kink solitons. Propagating solitons appear in two forms: The low energy form resembles standard solitons in anharmonic chains; the high energy form contains propagating flips. We discuss their stability and their contribution to energy transport.

MM 5: Interfaces I

Time: Monday 10:15–11:15 Location: H6

MM 5.1 Mon 10:15 H6

Stress Induced Migration of <100> Tilt Grain Boundaries in Al-Bicrystals — •Tatiana Gorkaya, Dmitri Molodov, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, 52056 Aachen

The stress induced migration of planar grain boundaries in aluminium bicrystals was measured. Both low- and high angle symmetrical <100> tilt grain boundaries with misorientation angles in the range between 3.5° and 23.0° were examined. Boundary migration under a shear stress was observed to be ideally coupled to the lateral translation of grains. The measured ratios of the normal boundary motion to the lateral displacement of grains are in an excellent agreement with the respective boundary geometry. The temperature dependence of grain boundary mobility was measured in the temperature range between 290°C and 390°C, and the corresponding activation parameters were determined. The activation enthalpy of boundary migration was found to be independent of misorientation angle in the investigated misorientation range and amounts to H=1.44 eV.

MM 5.2 Mon 10:30 H6

Influence of low angle grain boundaries on recrystallization — •Myrjam Winning — Max-Planck-Institut für Eisenforschung GmbH, Abteilung Mikrostrukturphysik und Umformtechnik, Düsseldorf, Germany

Recrystallization is one of the most effective ways to change the microstructure as well as the properties of crystalline materials. On one hand primary static recrystallization is defined by nucleation and growth, whereas the growth takes place by the motion of high angle grain boundaries. On the other hand it is known that even low angle grain boundaries are able to move and therefore able to contribute to microstructural changes. But although there is some experimental evidence that low angle grain boundaries can play a role during recrystallization the influence of low angle grain boundaries are usually not taken into account neither in experimental investigations nor in simulations of the recrystallization process.

In general, recrystallization models discriminate between three different types of grain boundaries: low angle grain boundaries which are immobile, random high angle grain boundaries which are mobile and sometimes also some special grain boundaries with a higher mobility than the random grain boundaries.

The aim of this study is to investigate the influence of mobile low angle grain boundaries on the microstructure and texture evolution during recrystallization of deformed Al single crystals by using a cellular automaton model.

MM 5.3 Mon 10:45 H6

Migration and Faceting of Low Angle Grain Boundaries in Aluminium-Bicrystals — •Bingbing Zhao, Dirk Kirch, Dmitri Molodov, and Günter Gottstein — Insitute of Physical Metal-

lurgy and Metal Physics, RWTH-Aachen University, Kopernikusstr. 14, 52056 Aachen, Deutschland

Migration and faceting behaviour of low angle <100> tilt grain boundaries in Al-bicrystals was investigated experimentally by in-situ observations in a scanning electron microscope. The results reveal that for grain boundaries with misorientation angles in the range $10°<\theta<15°$ there is a temperature TR, above which the boundary possess a curved shape and moves in a steady state under a capillary driving force. Below this temperature the grain boundary shows one singular facet corresponding to the minimum energy configuration with respect to the grain boundary inclination and does not move if the temperature remains constant. The transition temperature TR was found to depend on the misorientation angle θ. For boundaries with $\theta>15°$ no transformation faceted boundary-curved boundary was observed. At any temperature these boundaries moved in a steady state being curved. Also for boundaries with misorientations $\theta<10°$ no structural transition was observed. These boundaries keep their initial symmetrical straight configuration in the entire investigated temperature range up to the melting point of aluminium. The results are interpreted in terms of the grain boundary roughening transformation and the change of grain boundary properties in the transition range between low and high angle misorientations.

MM 5.4 Mon 11:00 H6

Modelling grains and bubbles: phase boundary evolution with volume constraints — Harald Garcke[2], Britta Nestler[1], Björn Stinner[3], and •Frank Wendler[1] — [1]University of Applied Sciences Karlsruhe, Moltkestr. 30, D-76133 Karlsruhe — [2]Department of Mathematics, University Regensburg, D-93040 Regensburg — [3]Department of Mathematics, University of Sussex, BN1 9RF, United Kingdom

In our talk we present a new phase-field model for the evolution of grain or bubble systems, where the motion of the interfaces is determined by the mean curvature and the volume of some or all of the phases is preserved. Based on previously published results [1] a multi-phase-field model of Allen-Cahn type is introduced wich includes nonlocal forcing terms. The phase boundary dynamics results from a gradient flow of a Ginzburg-Landau type energy and incorporates anisotropic surface energies and kinetics. The algorithms for the volume constraints and the numerical realization for a high number of phases are briefly presented. Simulation results are shown for 2D and 3D problems dominated by surface energy minimization like the formation of Wulff shapes, double crystals and bubble clusters. Wetting phenomena with a constant fraction of liquid phase are treated for cases where the bubble phase volume either is preserved (foams) or may change in time (solid/melt grain coarsening). Additional forcing terms due to a solid/liquid phase transition allow to simulate the inclusion of inert particles into a growing front.

[1] B. Nestler, H. Garcke and B. Stinner, Phys. Rev. E **71** (2005), 041609-1

MM 6: Interfaces II

Time: Monday 11:45–13:00 Location: H6

MM 6.1 Mon 11:45 H6

The role of quadruple points on grain microstructure evolution — •Volker Mohles, Luis Antonio Barrales-Mora, Lasar Shvindlerman, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, 52056 Aachen

It is well known that triple junctions between grains can have a significant influence on grain microstructure evolution. Now the effect of quadruple points on grain microstructure evolution has been investigated by computer simulations. For this purpose, a special grain assembly was employed. This special configuration allows a steady-state motion of the grain boundaries, permitting to study the effect of a finite mobility of the quadruple points on the evolution of the system. Numerous simulations, by means of a 3D Vertex Model, were performed varying the quadruple point mobility. The results of these simulations clearly demonstrate that quadruple points can drag grain growth kinetics. However, further simulations on the same configuration but for different triple junction mobilities showed that the dragging effect of triple junctions is considerably larger than the effect of quadruple points.

MM 6.2 Mon 12:00 H6

Bond-order potential for atomistic modeling of extended defects in tungsten — •Matous Mrovec[1,2], Christian Elsaesser[1,2], and Peter Gumbsch[1,2] — [1]IZBS, University of Karlsruhe, Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer-Institute IWM, Woehlerstr. 11, 79108 Freiburg

The bond-order potential (BOP) for transition metals is a real-space semi-empirical description of interactions between atoms, which is based on the tight-binding approximation and the d-band model. This scheme provides a direct bridge between the electronic-structure modeling and the atomistic modeling by coarse-graining the electronic degrees of freedom into a many-body interatomic potential. We will present a recently constructed BOP for the body-centered cubic transition metal tungsten. The potential was extensively tested against accurate DFT methods in order to assess its reliability and applicability. The high predictive power of the BOP will be demonstrated in studies of extended defects, namely low-index surfaces, symmetrical tilt grain boundaries, and lattice dislocations, which all affect the mechanical behavior of polycrystalline tungsten.

MM 6.3 Mon 12:15 H6

Untersuchung des Energie-Missorientierung-Phasenraums allgemeiner Cu-Korngrenzen — •Markus Ziehmer[1], Andreas Tschöpe[1], Carl Krill III[2] und Rainer Birringer[1] — [1]Technische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]Elektrotechnik, Universität Ulm, 89081 Ulm

Die spezifische Korngrenzenenergie γ ist von der Missorientierung $(\Theta,\vec{r})$ der angrenzenden Körner abhängig. Daraus resultiert ein Drehmoment, das unter der Voraussetzung ausreichender thermischer Aktivierungsenergie die Rotation der Körner in Richtung lokaler Energieminima antreibt.

Die Verbindung der etablierten Kugel-Platte-Methode mit der Orientierungsabbildenden Mikroskopie (OIM) bietet die Möglichkeit, die Rotation einzelner einkristalliner auf einem einkristallinen ebenen Substrat angesinterter Kugeln zu detektieren. Aus der Aufzeichnung der sich ändernden Missorientierung zwischen Kugel und Platte lassen sich Rückschlüsse über charakteristische Merkmale des $\gamma(\Theta,\vec{r})$-Phasenraums ziehen. Zusätzlich kann man unter der Annahme der Parallelität von Korngrenzenebene und Substratoberfläche die Tilt- und Twistanteile bestimmen.

Frühere Untersuchungen der Missorientierungsabhängigkeit von γ wurden meist an reinen Tilt- oder Twistkorngrenzen vorgenommen. Wir berichten über Messungen an allgemeinen Cu-Korngrenzen, die darauf hinweisen, dass die beobachteten Phänomene nicht durch das bisher verwendete einfache Bild des Energie-Missorientierung-Phasenraums adäquat beschrieben werden können.

MM 6.4 Mon 12:30 H6

Ab-initio based multiscale analysis of the 5D configurational space of Grain Boundaries in Aluminum. — •Liverios Lymperakis and Jörg Neugebauer — Computational Materials Design department, Max-Planck-Institut für Eisenforschung, Düsseldorf

A rapidly evolving approach in materials design is Grain Boundary (GB) engineering, i.e. optimizing the population of GBs with desirable geometry by suitable thermomechanical treatment. To achieve this, a deeper understanding and quantification of the interplay between the GB energies with respect to the misorientation of the two grains (3 dimensional configuration space) and the inclination of the boundary plane (2D space) are crucial. In this work we combine first principles density functional theory with modified embedded atom method (MEAM) calculations in order to explore the 5D-phase space of GBs in Aluminum. To handle this problem, we have generalized our implicit boundary multiscale schema (IBMS) which had been originally developed and applied to study isolated dislocations [1]. In a first step we have explored the three degrees of freedom required to describe the misorientation of the two grains: as an example we discuss symmetri-

cal tilt GBs having the rotational axis along high symmetry directions of the fcc lattice. As a second example we focus on the low energy misorientation angles and explore the remaining two degrees of freedom associated with the inclination of the boundary plane. These results have been able to interpret and explain recent experimental data on GB occupation [2]. [1] L. Lymperakis et al. Phys. Rev. Lett. 93, 196401 (2004). [2] C.-S. Kim et al. Scripta Materialia 54, 1005 (2006).

MM 6.5 Mon 12:45 H6

Simulations of grain coarsening considering complex energy dependences — •Yingxiao Ma, Volker Mohles, Luis Antonio Barrales-Mora, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, 52056 Aachen

The energy of grain boundaries in metals depends on their geometrical parameters (misorientation and inclination) in a complex manner. A function is proposed which allows to describe this energy dependence in a rather convenient way for engineering purposes. It is based on the idea of special large angle boundaries (sigma boundaries) being superimposed with small angle boundaries, in order to describe general boundaries. The energy of the small angle part is derived from dislocation theory, whereas the high angle part may be derived from atomistic simulations. Applying this energy function, the 2D vertex dynamics model is used to simulate grain growth in Aluminium. Microstructure evolution, grain growth kinetics, the von Neumann-Mullins relation and the distributions of grain size and misorientation in 2D polycrystals have been examined. The sensitivity of the results on the initial conditions (experimental/random orientations) and on the details of the energy function is determined.

MM 7: HV Greer

Time: Monday 14:00–14:30 Location: H16

Invited Talk MM 7.1 Mon 14:00 H16

Metallic Glasses — •Lindsay Greer — Dep. of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, UK

Metallic glasses of many different compositions are now available in bulk (with minimum dimension of more than 1 cm). This has excited interest in these glasses as structural materials, and indeed they do show exceptionally high strength and capacity for elastic-energy storage. They suffer from very limited plasticity, and there has consequently been much interest in the mechanisms of their plastic flow. This presentation deals first with why metallic glasses are attractive for a wide variety of structural and device applications, and then focuses on the emerging understanding of their plastic deformation. Under normal testing conditions, plastic deformation in these glasses is sharply localized into shear bands only 10 nm thick. The extreme conditions in these bands are a focus of current research. Already it is clear that there are very good correlations — much better than for crystalline metals — between elastic properties, plasticity and glass-forming ability.

MM 8: SYM Micro- and Nanomechanics II

Time: Monday 14:45–17:00 Location: H16

MM 8.1 Mon 14:45 H16

Superplastic deformation of ultrafine-grained Mg-alloys produced by micro-alloying and equal channel angular extrusion — •Florian H. Dalla Torre[1], Anja Hänzi[1], Maciej Krystian[2], Peter J. Uggowitzer[1], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Wolfgang-Pauli-Str. 10, 8093 Zürich, Switzerland — [2]ARC Seibersdorf Research GmbH, Materials Research , Materials Micro-/Nanoengineering

The 'grain growth restriction'- concept via the addition of elements such as Zn, Ca, and Zr to Mg was used to cast and extrude two alloys with grain sizes of <5 and <10 micrometers, respectively. In combination with equal channel angular extrusion processing, the grain size was further reduced. Mechanical testing showed a substantial increase in ductility at room temperature compared to that in conventional Mg alloys. In addition, the high strain rate sensitivity, in combination with the effect of micro-alloying elements on stabilizing the grain size yields beneficial properties for superplastic micro- and net-shape-forming processes. The dependence of texture, grain size and twinning is discussed, together with their influence on temperature-dependent deformation mechanisms.

MM 8.2 Mon 15:15 H16

Deformation Processing of Massive Nanostructured Materials — •Gerhard Wilde — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

One way to obtain massive specimens, e.g. of pure fcc or hcp metals with extremely small average grain sizes is given by repeated cold-rolling, as shown recently for several pure metals. In fact, even intermetallic alloy phases with rather high melting temperatures could be processed successfully, such that a residual grain size of less than 100 nm was obtained. This new method extends the range of microstructures that are accessible by severe plastic deformation treatments towards smaller grain sizes. In contrast to nanocrystalline materials obtained by powder methods such as inert gas condensation, the material synthesized by cold rolling contains a high density of dislocations as well as significant residual strain in the nanosized grains. In addition, to synthesis, recent results related to the underlying deformation mechanisms of the nanocrystalline material containing lattice defects as well as new measurements of the mechanical properties hardness and strength in dependence of the grain size and will be discussed for pure fcc model systems. These first results indicate significant improvements concerning properties and performance that can be gained through nanostructuring by applying advanced deformation processing treatments. The ongoing work is supported by the Deutsche Forschungsgemeinschaft.

15 min break

MM 8.3 Mon 16:00 H16

Strain-Rate-Sensitivity of nanocrystalline Ni investigated with nanoindentations and compression tests — •Johannes Mueller and Mathias Göken — Institut für Werkstoffwissenschaften, Universität Erlangen-Nürnberg

The deformation behaviour of nanocrystalline materials is known to be dependent of the deforming strain rate. The reason for this strain-rate-sensitivity is subject to ongoing research. An technologically interesting field is coating of components with thin layers. Nanoindentation is a suitable method to characterise mechanical properties of those thin coatings. However the data obtained by nanoiondentation is not trivially comparable to those obtained by macroscopical method. In this work the strain-rate-sensitivity of nanocrystalline electrodeposited nickel is studied using compression tests and nanoindentations using different indenter shapes. Explanations for the differences found, are discussed.

MM 8.4 Mon 16:15 H16

A nanomechanical approach to hydrogen embrittlement of metals — •Afrooz Barnoush and Horst Vehoff — Saarland University, Department of Materials Science, Bldg. D22. P.O. Box 151150, D-66041 Saarbruecken, Germany

New nanomechanical testing methods like nanoindentation allows us to study mechanical properties of materials in nano scale where the plas-

tic deformation could be studied in detail. This was the motivation for a nanomechanical approach to hydrogen embrittlement of metals using a novel in-situ electrochemical nanoindentation setup. In this work nanoindentation has been used to study the effect of hydrogen on deformation of small volumes for nickel and copper single crystals as two metals with different sensitivity to hydrogen embrittlement. Nickel is known to be prone to hydrogen embrittlement where there is no hydrogen embrittlement for copper. Electrochemical hydrogen charging reduces the load at which dislocations are nucleated (pop-in load) in nickel, while this results in no observable change in the pop-in load of copper single crystal as expected. The experimental results are analyzed using a thermodynamic model for homogenous dislocation nucleation. Based on these analyses, the activation energy for the onset of plasticity is believed to be reduced by the dissolved hydrogen in crystal lattice.

MM 8.5 Mon 16:30 H16

Plasticity of thin polycrystalline metallic films: a discrete dislocation dynamics approach — •Jochen Senger[1], Daniel Weygand[1], Oliver Kraft[1,2], and Peter Gumbsch[1,3] — [1]IZBS, Universität Karlsruhe (TH) — [2]IMF II, Forschungszentrum Karlsruhe — [3]IWM, Fraunhofer Institut für Werkstoffmechanik, Freiburg

Recent experimental observations (Spolenak et al, PRL 90, 096102, 2003) showed that the stress distribution in polycrystalline thin metal films upon thermal cooling or heating can be quite inhomogeneous. Stress variations were observed between grains and even within grains. To study such stress distributions, a parallel discrete dislocation dynamics (DDD) tool is employed, based the tool described in Weygand et al., Mod. Sim. Mater. Sci. Eng. 10 (2002) 437. The parallelization is achieved using OpenMP for shared memory platforms. The concept is based on a common data structure, where the individual calculation tasks are distributed among the CPUs. The main computational tasks, the interaction calculation between dislocation and the evaluation of the boundary conditions are performed on multiple CPUs and a very good scaling is achieved. The parallelized version of the DDD code is applied to the simulation of the small scale plasticity of polycrystalline thin films. The dislocation microstructure evolution and the resulting stress distributions are analysed and compared experiments and single grain simulations. If the calculated stresses of the multi grain simulations are averaged over areas corresponding to the experimental resolution, excellent agreement is found for stress amplitudes in simulation and experiment.

MM 8.6 Mon 16:45 H16

Modulated lateral force microscopy: an AFM tool for analysis and modification of polymer surfaces — •Heinz Sturm — BAM VI.25, Federal Institute for Materials Research, Unter den Eichen 87, D-12205 Berlin

Scanning Probe Microscopy, here Scanning Force Microscopy in the contact mode, is widely used not only to examine the 3-dimensional surface topography, but also to evaluate nano-mechanical surface properties. This contribution focuses on the tip-surface interaction due to a shear deformation, i. e., friction. During forward and backward scan with a given scanning (shear) velocity, the cantilever lateral bending (torsion) is a measure for the lateral force. Unfortunately, both scan directions must be acquired and subtracted to separate the topography cross-talk from the friction image. Superimposing a lateral displacement between tip and surface via a dither piezo, the shear deformation is sinusoidally modulated. Images of amplitude and phase shift of the dynamic cantilever torsion within a frequency range from 30 kHz up to 60 MHz are presented. Due to the fact that friction is always a dynamic process, we prefer to call this technique "Modulated Lateral Force Microscopy" (MLFM) instead of just "Dynamic Friction Microscopy". The dependence of the modulated friction from the normal force between tip and lever can be described with the Johnson-Kendall-Roberts model.

MM 9: Liquid and amorphous materials III

Time: Monday 14:45–15:45 Location: H4

MM 9.1 Mon 14:45 H4

Liquid phase demixing and growth in Cu-based alloys — •Matthias Kolbe[1], Jianrong Gao[2], Jiuzhou Zhao[3], Lorenz Ratke[1], and Dieter Herlach[1] — [1]DLR, Institut für Materialphysik im Weltraum, Linder Höhe, 51170 Köln — [2]Key Lab of Electromagnetic Processing of Materials, North Eastern University, Shenyang 110004, China — [3]Institute of Metal Research, CAS, Shenyang 110016, China

Cu-based alloys as Cu-Cr, Cu-Co, Cu-Nb and Cu-Fe exhibit a flat liquidus in the binary phase diagram. This property is often associated to metastable phase separation in the region of the undercooled melt: When the metastable miscibility gap is entered, the homogeneous alloy separates into a Cu-rich and a Cu-poor liquid. The undercooled melt solidifies rapidly and the metastable liquids are frozen in. Microstructure analysis of the solidified material allows the determination of properties of the metastable liquids. We studied phase separation and phase growth of the metastable Co-rich L1 phase in Co-84at%Cu by electromagnetic levitation (EML) and drop tube experiments. In addition, samples have been processed and solidified in the TEMPUS facility during parabolic flights under low gravity conditions. Compared to processing in EML on ground, the fluid flow is reduced in TEMPUS by an order of magnitude. The solidified microstructures show the influence of cooling rate and of the different convection levels in the liquid on phase growth. The results are discussed within current models of liquid phase growth.

MM 9.2 Mon 15:00 H4

Negative entropy of mixing in computer simulated bulk glass forming AlxNi1-xZr60 melts — Mohammed Guerdane and •Helmar Teichler — Inst. f. Materials Physics, University of Göttingen, D-37077 Göttingen

For multi-component random systems, the ideal solution model predicts positive entropy of mixing, reflecting the increase of configuration space by exchange of chemically different particles. Glass forming melts are usually far from being random. Regarding this, AlxNi1-xZr60 is known to have marked short- and intermediate-range order. The former is characterized by icosahedral neighbour cages around Al- and by trigonal-prismatic ones around Ni-atoms, the latter by chain arrangements of Al- and of Ni-cages (M. Guerdane and H. Teichler, PRE 65, 014203 (2001)). Here the question arises whether in AlxNi1-xZr60 melts the entropy of mixing is positive, due to a gain in configuration space by particle exchange, or negative, due to a decreased density of low-energy states in the complex liquid at mid-concentrations. Concerning this, we report molecular dynamics results for AlxNi1-xZr60 melts based on the adiabatic switching approach. They show strong negative entropy of mixing along the quasi-binary line, i.e., predominance of enthalpic over entropic effects in this bulk glass forming liquid. (Supported by DFG SPP 1120 *Phase Transformations in Multi-Component Melts*.)

MM 9.3 Mon 15:15 H4

Primary crystallization reaction in Al-Y-Fe glasses containing low melting point nanoparticles — •Nancy Boucharat[1], Harald Rösner[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, P.O.B. 3640, 76021 Karlsruhe, Germany

Many rapidly quenched Al-rich alloys partially devitrify via a primary crystallization reaction, which results in the development of a high num-ber density of homogeneously dispersed Al-nanocrystals. Although sev-eral experimental results are consistent with the formation of nucleation sites during rapid quenching via homophase catalysis, the nature and the origin of the nucleation sites is not yet completely resolved. To assess the role of the as-quenched state in the nanocrystallization process, 1at.% Pb or 1at.% In, respectively were substituted for Al in an Al-Y-Fe glass prior to rapid quenching. The microstructure of the respective products consists of a homogeneous dispersion of nanocrystalline Pb particles or In-enriched regions within an amorphous Al-Y-Fe matrix. In both cases, the primary crystallization is strongly shifted to lower temperatures compared to the reaction in the inclusion-free sample. While likely mechanisms have been proposed

to explain the catalytic effect of Pb inclusions on the nanocrystallization process, the analyses on the In-containing sample give new evidence that the inclusions generate a modification of the local structural arrangement of the amorphous matrix promoting the retention of quenched-in nuclei during the quenching process.

MM 9.4 Mon 15:30 H4

Microstructure and properties of glassy NdCoAl alloys with Ga and Nb additions — •Mihai Stoica[1], Mihaela Buschbeck[2], Annett Gebert[2], Ludwig Schultz[2], Albrecht Wiedenmann[3], Olivier Perroud[3], Shankar Wenkataraman[1], Simon Pauly[1], and Jürgen Eckert[1] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270016, D-01171 Dresden, Germany — [2]IFW Dresden, Institute for Metallic Materials, P.O. Box 270016, D-01171 Dresden, Germany — [3]Hahn-Meitner Institute Berlin, Glienickerstr. 100, D-14109 Berlin, Germany

The glass forming ability and structure upon fast cooling were investigated for Nd60Co30Al10 with Ga and Nb additions. The investigated alloys contained 1, 3 and 5 at. % of Ga or Nb. From every composition different samples were produced. The melt spinning apparatus was used to make glassy ribbons 4 mm wide and 0.03 mm thick and by copper mould casting rods with diameters of 1 and 2 mm were cast. The structure of the samples was investigated by means of X-ray diffraction and electronic microscopy and the thermal stability by differential scanning calorimetry (DSC). In order to rule out the effect of composition and cooling conditions, the microstructure and thermal behaviour of master alloys with and without Ga and Nb additions were also checked. The paper will discuss the microstructure formation for different samples, as a function of two parameters: the composition and the cooling rate. The work was supported by the German Science Foundation (DFG) via the DFG priority program *Phasenumwandlungen in mehrkomponentigen Schmelzen*.

MM 10: Liquid and amorphous materials IV

Time: Monday 16:15–17:30 Location: H4

MM 10.1 Mon 16:15 H4

Structure and electronic transport of *a*-$Ni_x(Ti_{50}Al_{50})_{100-x}$ — •Jan Rauchhaupt, Thomas Raubold, and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

An approach to understand the development of any crystalline structure from the initial disordered state is to investigate stabilization processes in amorphous phases as precursors of any ordered structure. Amorphous thin films are ideal to do so because they exist in just one phase, can be prepared in exactly the right composition and the development of their structure and electronic transport properties dependent on the composition and temperature are easy to measure. In order to minimize their global energy many different alloys organize themselves under the influence of a resonant interaction between the valence electrons as one subsystem and the static structure as the other one. These resonances were observed in many systems, from simple metals and semiconductors to ionic glasses and TM-containing alloys (TM=transition metal). We discuss the results of the measurements as a hybridization effect of the Al-p-electrons with the empty d-states of the TM. Amorphous ternary alloys of Ni, Ti and Al were prepared in situ at T=4 K in a HV-cryostate and were annealed up to the crystalline state. The static structure, by means of electron diffraction, the resistivity and the thermopower were measured as a function of temperature and composition. Additionally quantitative *White Lines* measurements were performed to prove the predicted hybridization effects.

MM 10.2 Mon 16:30 H4

FeNbB bulk metallic glass with high boron content — •Mihai Stoica[1], Khalil Hajlaoui[2], Jayanta Das[1], Jürgen Eckert[1], and Alain Reza Yavari[2] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270016, D-01171 Dresden, Germany — [2]LTPCM-CNRS, I.N.P. Grenoble, 1130 Rue de la Piscine, BP 75, F-38402 University Campus, France

Fe-based alloys able to form magnetic bulk metallic glasses (BMGs) are of the type transition metal – metalloid and often contain 5 or more elements. Usually, the metalloid content is around 20 atomic %. Very recently, the Fe66Nb4B30 alloy was found to be able to form BMG by copper mold casting technique, despite its high metalloid content. Several composition with boron contents around 30 at. % or even higher were calculated since 1993 as possible compositions of the remaining amorphous matrix after the first stage of nanocrystallization of Finemet-type Fe77Si14B9 glassy ribbons with 0.5 to 1 atomic % Cu and a few percent Nb addition. Melt-spun ribbons of all calculated compositions were found to be glassy. The composition of the ternary Fe-based BMG investigated in the present study resulted as an optimization of all possibilities. The alloy is ferromagnetic with glass transition temperature Tg = 845 K, crystallisation temperature Tx = 876 K, liquidus temperature Tliq = 1451 K and mechanical strength of 4 GPa. The coercivity of as-cast samples is very low, around 1.5 A/m. The present contribution aims at discussing the thermal stability, mechanical and magnetic properties of the Fe66Nb4B30 BMG.

MM 10.3 Mon 16:45 H4

Microstructure of rapidly quenched amorphous Ni100-2xNbxYx alloys — •Norbert Mattern[1], Uta Kuehn[1], Thomas Gemming[1], Guenter Goerigk[2], and Juergen Eckert[1] — [1]Leibniz-Institut IFW Dresden, Helmholtzstr.20,01069 Dresden — [2]Haysylab at DESY,Notkestr.85,22603 Hamburg

Two-phase amorphous Ni-Nb-Y alloys can be prepared by rapid quenching from the melt[1]. The structure formation takes place in the phase separated undercooled liquid. Recent experimental and thermodynamical assessment of the Ni-Nb-Y phase diagram shows an extension of miscibility gap in the melt of the monotectic binary Nb-Y system up to 60 at% Ni content into the ternary Ni-Nb-Y system.The microstructure of the as-quenched ribbons consists of two amorphous regions Nb-enriched and Y-enriched exhibiting features of self-similarity with a size distribution from micrometer dimensions down to several nanometers. Small-angle X-ray diffraction confirms the fractal microstructure. For Ni contents > 60at% (critical composition) a "homogeneous" amorphous microstructure is observed by transmission electron microscopy (TEM) in accordance with thermodynamic calculations which are based on the regular solution model for the liquid. On the other hand, small-angle X-ray diffraction data indicate clearly chemical inhomogeneities within the nm-range. From the inhomogeneous amorphous precursors ultrafine nanocrystalline microstructure can be formed upon annealing as the first step of crystallization.

[1]N. Mattern, U. Kuehn, A. Gebert, T. Gemming, M. Zinkevich, H. Wendrock, L. Schultz, Scripta Mater., 53 (2005) 271

MM 10.4 Mon 17:00 H4

Cold rolling induced amorphization and nanocrystallization processes studied by positron lifetime and 2-dimensional Doppler broadening measurements — •Wolfgang Lechner[1], Werner Puff[1], Herbert Rabitsch[1], Gerhard Wilde[2], and Roland Würschum[1] — [1]Institut für Materialphysik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria — [2]Institut für Materialphysik, Universität Münster

In order to contribute to an atomistic understanding of the interfacial structure and processes during amorphization and nanocrystallization, the present work deals with studies of interfacial free volumes by means of positron-annihilation-spectroscopy. In addition to positron lifetime spectroscopy, coincident Doppler broadening of the positron-electron annihilation photons is applied as novel technique for studying the chemistry of interfaces. To study the amorphization process, pure foils of Cu and Zr with a nominal composition of $Cu_{60}Zr_{40}$ were mechanically intermixed by cold rolling. Starting from the constituent pure metals, a nanoscale multilayer structure of elemental layers and amorphous interlayers develops in an intermediate state of folding and rolling, where free volumes with a Zr-rich environment occur that are presumably located in the hetero-interfaces between the various layers or in grain boundaries of the Cu-layers. To analyze the nanocrystallization reaction that occurs in marginal glass formers, pure foils of Al and Sm with a composition of $Al_{92}Sm_8$ were produced by the abovementioned synthesis route. Specific modifications of free volumes and their chemical environment could be observed for various strain levels.

MM 10.5 Mon 17:15 H4

Nanocrystallisation of amorphous Al85Ni10La5 powder induced by severe plastic deformation — •Jens Vierke[1], Vitaly Pilyugin[2], Ingwer Denks[1], Nelia Wanderka[1], Markus Wollgarten[1], and John Bahnhart[1] — [1]Hahn-Meitner-Institute Berlin, Glienicker Str. 100, 14109 Berlin, Germany — [2]Russian Academy of Sciences, Institute of Metal Physics, Kovalevray street 18, 620219 Yekaterinburg, Russia

The nanocrystallisation behaviour of Helium-atomised amorphous Al85Ni10La5 powder subjected to high pressure torsion (HPT) at room temperature and thermal treatments have been studied by differential scanning calorimetry (DSC), wave- and energy-dispersive X-ray diffraction and scanning and transmission electron microscopy. DSC experiments combined with X-ray diffraction analysis show a joint precipitation of α-Aluminium and intermetallic phases at an onset temperature of 276°C, using a heating rate of 40 °C/min. On the contrary, a primary precipitation of α-Aluminium was observed in powders which were deformed by HPT at room temperature. X-ray diffraction analysis of HPT-discs shows that a rising shear deformation leads to a growing number of Al-nanocrystals in the amorphous matrix. The presented results are discussed regarding the development of the microstructure during the consolidation of this powder.

MM 11: Interfaces III

Time: Monday 14:45–15:45 Location: H6

MM 11.1 Mon 14:45 H6

Carbide precipitation at a grain boundary in molybdenum - an ab-initio DFT study — •Rebecca Janisch[1] and Christian Elsässer[2] — [1]Universität Erlangen-Nürnberg, Institut für Werkstoffwissenschaften (WWI), Martensstr. 5, 91058 Erlangen, Germany — [2]Fraunhofer-Institut für Werkstoffmechanik, Wöhlerstr. 11, 79108 Freiburg, Germany

Atomic-scale stages of the growth of an interfacial precipitate film of tetragonal molybdenum carbide at a $\Sigma 5$ (310) [001] symmetrical tilt grain boundary in molybdenum were investigated by means of atomistic supercell calculations on the basis of ab-initio density functional theory (DFT). In this presentation, the structural development of the precipitate with increasing carbon concentration is analysed. The structurally optimised atomistic model for the fully developed precipitate is compared to experimental high-resolution images from transmission electron microscopy, and it allows to clarify some ambiguous features therein. An atomic-scale twinning mechanism in the MoC precipitate is proposed. Finally, the influence of the carbon concentration on the stability of the metal-carbide interface with respect to cleavage is discussed.

MM 11.2 Mon 15:00 H6

The role of crystallography in topotaxial first-phase selection — •Andriy Lotnyk, Stephan Senz, and Dietrich Hesse — Max Planck Institute of Microstructure Physics

The role of crystallography in topotaxial first phase formation in the MgO-TiO_2 system is studied. The question which phase forms first in a thin-film solid state reaction, if the corresponding phase diagram permits the formation of several phases, is of considerable scientific and technological significance. Correspondingly, a number of models have been put forward, including kinetic, thermodynamic, and nucleation-related models. In the present work, vapor-solid reactions between MgO (vapor) and TiO_2 (rutile) single crystals with different surface orientations were performed. The crystallographic relations between the product phases and the TiO_2 substrates were studied by X-ray diffractometry and transmission electron microscopy. A topotaxial formation of $MgTiO_3$ on the rutile crystals was found. Previous results on vapor-solid reactions of TiO_2 (vapor) with MgO substrates showed the topotaxial formation of Mg_2TiO_4. We conclude that in the MgO-TiO_2 system, in case of a topotaxial solid state reaction, the phase forming first depends on the crystallography of the substrate serving as reactant. Thus, crystallography obviously can play an important role in the determination of the first growing phase in topotaxial solid-state reactions.

MM 11.3 Mon 15:15 H6

Al-Al Compound Casting — •Konrad Papis, Peter Uggowitzer, and Jörg Löffler — ETH Zurich, Laboratory of Metal Physics and Technology, Zurich, Switzerland

'Compound casting' is a process where a melt is cast onto or around a solid metallic 'insert'. It is the realization of a simple joining procedure for light metals aimed at weight-saving. Difficulties inherent in joining aluminium are its natural oxide layer and the formation of intermetallic phases. In this project, both the solid substrate and the melt used are aluminium alloys containing various alloying elements (Cu, Si, Zn in the melt, Mg in the substrate). Compounds with flawless interfaces (no contraction defects, no oxides) were successfully produced by replacing the oxide layer with a zinc layer. This was accomplished by pickling the substrate in a solution containing zincate ions, implying a redox reaction by which zinc is deposited in its metallic form. The composition and mechanical properties of the compounds' interfacial regions were investigated by SEM/EDX and microhardness measurements following the 'compound casting' process and successive heat treatments. DICTRA calculations were carried out to simulate the diffusion processes at the interface. The results from the mechanical characterization were compared to the simulations, the conclusion being that diffusion of alloying elements led to precipitation hardening of the compound.

MM 11.4 Mon 15:30 H6

Investigation of Fe/MgO interfaces by Atom Probe Tomography (APT) — •Alexander Mackel, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

Modern magnetic storage devices such as Magneto-resistive RAM (MRAM) devices are generally built up from a stack of thin layers, in which one of these layers is an oxide-barrier. The effect of Tunnelling Magneto-Resistance (TMR), governing the function of these devices, is strongly dependent on the electron transmission, in particular, at the Oxide/Metal interface. Therefore, it becomes important to characterize these interfaces on the nano-scale concerning their geometrical and chemical roughness. With this objective, we investigated the stacking of an ideal Fe/MgO/Fe sandwich type by means of APT.

The layers were prepared by ion beam sputtering on tungsten substrate-tips of 30 to 50nm radius of curvature as well as on Si-posts with a planar surface. Using a Focused Ion Beam, these posts were formed into a needle-like shaped tip to enable APT investigation.

The model system has been analyzed successfully for barrier thicknesses smaller than 2nm. So far, we found a FeO-peak in the time-of-flight mass spectrum of the interface indicating that Fe is partly oxidized already in the as-prepared state. The origin and presence of the FeO will be discussed as well as a comparison between the results obtained from both types of samples.

Financial support by the Deutsche Forschungsgemeinschaft, SFB602/B1 is gratefully acknowledged.

MM 12: Growth

Time: Monday 16:15–17:45 Location: H6

MM 12.1 Mon 16:15 H6

Growth History of Single Grains in 3D Normal Grain Growth — •Dana Zöllner and Peter Streitenberger — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Materialphysik, PF 4120, D-39016 Magdeburg

A 3D grain growth model is presented, which allows the prediction of the growth history of single grains. The model is based on a generalised mean-field approach resulting in an analytic grain size distribution function that represents the data of three dimensional grain growth - simulated with a large 3D Monte Carlo Potts model algorithm - very well. The parameters from the obtained grain size distribution are then used to calculate an analytic function representing the further growth history by showing the temporal development of the grain radius for a fixed but selectable initial grain size. The results are compared with the 3D Monte Carlo simulation giving very good agreement. Furthermore, the life spans of single grains are calculated as a function of their size showing again a good agreement with the simulation results.

MM 12.2 Mon 16:30 H6

Abnormal grain growth of nanocrystalline materials: In situ investigation in the SEM — •Michael Marx, Andreas Noll, and Horst Vehoff — Saarland University, Materials Science, Building D22, 66041 Saarbrücken, Germany

To develop nanocrystalline (NC) and ultra fine grained (UFG) materials to secure operating construction materials, it is essential to stabilize the microctructure. So far the different mechanisms of grain growth and recrystallization were often investigated however a final description through all stages of grain growth is missing. Therefore in this work NC und UFG materials which were produced by different procedures were imaged in a SEM during heat treatment. The materials investigated were pulse electro deposited (PED) nickel, severe plastic deformed (SPD) aluminium by equal channel angular pressing for 2 and for 8 passes and an AlMgSi-alloy produced by accumulative roll bonding also for 2 and for 8 passes. No significant difference in the development of the microstructure between PED and SPD materials was found. In every case there is abnormal grain growth which results in an UFG matrix with some large grains of more than 100 um, the ratio of matrix grains and larger grains varies with the heat treatment. The growth of the large grains was monitored and the growth kinetics measured. By focused ion beam combined with orientation imaging microscopy, the growing grain boundaries could be identified as (100)-planes. So far the investigations are not finished however it will not be easy to find a heat treatment to produce a mono-modal ultra fine grained microstructure which is stable at moderate temperatures.

MM 12.3 Mon 16:45 H6

In situ investigation of Ostwald ripening in Al-Cu alloys by x-ray microtomography — •Mehdi Lalpoor[1], Lukas Helfen[2], and Carl Krill[1] — [1]Institute of Micro and Nanomaterials, Ulm University, D-89081 Ulm — [2]Institut für Synchrotronstrahlung (ISS/ANKA), Forschungszentrum Karlsruhe, D-76021 Karlsruhe

Conventional methods for studying Ostwald ripening in multiphase alloys rely on the characterization of planar sections, which provide access to statistically averaged microstructural parameters but not to local quantities, like the actual 3D shapes of individual particles. Serial sectioning can capture the 3D microstructure of solid specimens, but it destroys them in the process, rendering the procedure unsuitable for *in situ* coarsening studies. In contrast, x-ray microtomography delivers 3D microstructural data in a nondestructive manner, thus providing a way to track sample evolution over time. We report a first application of this approach to Ostwald ripening occurring in the model system Al-6.7 wt% Cu above its eutectic temperature. A temporal sequence of absorption-contrast tomographic images reveals the growth/shrinkage of solid α-Al particles embedded in a liquid phase richer in Cu. Microstructural evolution is found to be a superposition of coarsening-driven migration of phase boundaries and gravity/thermal gradient-driven vertical displacement. Quantitative values for local and global coarsening rates are extracted via image segmentation and combined with the results of conventional 2D studies to obtain additional insight into the influence of the volume fraction of the coarsening phase on the kinetics of Ostwald ripening in this system.

MM 12.4 Mon 17:00 H6

Modeling of equiaxed solute-controled dendrites which interact via a temperature* field — •Matthias Jurgk[1], Heike Emmerich[2], and Ricardo Siquieri[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Institut für Gesteinshüttenkunde, Rheinisch-Westfälische Technische Hochschule, Aachen, Germany

A fundamental challenge in the modeling of solidification processes arises from the many different length scales, on which important subprocesses take place.

We discuss a model for dendritic microstructures in the solidification of binary alloys. For most alloys the transport scales of solute diffusion and heat diffusion differ by several orders of magnitude. The two-scale model, which we discuss, includes both these transport scales in an efficient manner and enables us to study a whole array of equiaxed dendrites, whose microstructure morphology is controled by the slow solute transport but which interact with each other via the fast temperature transport.

One crucial parameter of the model is the ratio of both transport scales. Our numerical investigations of the model indicate the existence of two different growth regimes of the dendrites in dependence on the ratio of the transport scales. Another important parameter in the model is the density of the dendritic nuclei in the considered domain. We will also discuss the influence of this density on the growth dynamics of the dendritic microstructures.

MM 12.5 Mon 17:15 H6

Recrystallisation phenomena of HPT-processed 99.99% iron. — •Kejing Yang[1], Ralf Theissmann[2], Julia Ivanisenko[2], and Hans-Jörg Fecht[1,2] — [1]Materials Division, University of Ulm, 89091 Ulm, Germany — [2]Institut für Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

The understanding of mechanisms governing the recrystallisation of nanocrystalline metals and alloys is important for fundamental materials science, but also for practical applications of such materials, because it can help to find out the routs for improvement of their thermal stability. We conducted a comprehensive investigation of microstructure evolution upon annealing in the temperature range between 100°C and 400°C of high purity (99.99%) iron processed by severe plastic deformation using transmission and orientation imaging microscopy, and XRD analysis. The as-processed microstructure was typical of severely deformed metals consisting of grains with a mean size of 160 nm, and subgrains with a mean size of 90 nm. The grain boundaries originated from plastic deformation are in non-equilibrium state, which is manifested in presence of steps and facets in their structure, and a high level of micro stresses of 0.2 %. After annealing at 200°C for 1 hour, a growth of both grains and subgrains was observed, and after 400°C the microstructure was completely recrystallised. The mechanism of recrystallisation of as-processed iron was of continuous type. Surprisingly, a very high dislocation density was observed in grains after recrystallisation. Presumably, these dislocations appeared as a result of migration of grain boundaries with steps.

MM 12.6 Mon 17:30 H6

Kinetics of grain growth in nanocrystalline Fe at low annealing temperatures — •Heiko Paul and Carl Krill — Institute of Micro and Nanomaterials, Ulm University, D-89081 Ulm

At low annealing temperatures the rate of grain growth observed in nanocrystalline materials can be orders of magnitude smaller than would be expected from an extrapolation of high-temperature growth recorded in coarse-grained counterparts. One possible explanation for this observation rests on the drag force exerted on moving grain boundaries by triple junctions (TJ), the migration rate of which is independent of the average grain size $\langle R \rangle$ [1]. Since the curvature-driven speed of a grain boundary (GB) varies inversely with $\langle R \rangle$, there must be a critical grain size below which TJ migration becomes the rate-controlling step for grain growth. Likewise, if the activation enthalpy for triple-junction migration is higher than that of grain boundaries, then low annealing temperatures should favor TJ-controlled growth. We have searched for the latter by carrying out long-term *in situ* investigations of coarsening in high-purity nanocrystalline Fe at temperatures as low as 470°C. Grain growth was measured in a laboratory

x-ray diffractometer equipped with a high-temperature chamber and position-sensitive detector. An automated analysis routine was developed to extract the average grain size and microstrain from wide-angle diffraction scans, yielding isothermal grain-growth curves of unprecedented accuracy and duration for a nanocrystalline specimen.

[1] U. Czubayko, V. G. Sursaeva, G. Gottstein and L. S. Shvindlerman, *Acta mater.* **46** (1998) 5863–5871.

MM 13: HV Yip

Time: Tuesday 9:30–10:00 Location: H16

Invited Talk MM 13.1 Tue 9:30 H16

Computational Materials — •Sidney Yip — Department of Nuclear Science and Engineering and Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139-4307 (USA)

Computational science – the use of advanced computing capabilities to solve complex problems – has become critical to all scientific and technological endeavors in our society, whether it is for scientific leadership as in universities, for economic competitiveness in corporate research laboratories, or for national security in government agencies. At the intersection of computational science and materials research is a sweetspot for the physics community, offering fundamental challenges as well as technologically relevant applications. This talk will examine the role of multiscale modeling and simulation in providing insights to mechanical and thermal behavior of condensed matter, with a view towards materials characterization and design. A central theme is shear stability and localization which manifest in considerations of theoretical strength of crystals, thermodynamic versus mechanical melting, solid-state amorphization, and brittle to ductile transition in fracture. Another theme is thermal and electron transport in a class of problems which combine chemical physics with materials science. These investigations pave the way to tackling even more complex phenomena in materials the technological significance of which is quite transparent, such as viscous flow of molten glass, hardening kinetics of cement paste, and deformation of tempered steel in fatigue.

MM 14: SYM Micro- and Nanomechanics II

Time: Tuesday 10:15–12:15 Location: H16

Invited Talk MM 14.1 Tue 10:15 H16

Micromechanics inside the SEM — •Benedikt Moser — Empa, Materials Science and Technology, 3602 Thun, Switzerland

A large variety of in-situ mechanical experiments have been developed over the last 10 years in a number of research institutes. Many of those experiments can be performed inside the scanning electron microscope, some of them even in the transmission electron microscope (JMR (2005) July issue). These techniques offer a wealth of new information on small scale deformation mechanics to the scientists and may avoid some measurement artefacts in difficult experiments by visual control. In this presentation the author will discuss two examples of in-situ micromechanical experiments based on a custom-built micro-indentation apparatus adapted to a standard scanning electron microscope.

The first part will discuss the in-situ indentation of a metallic glass. Here the formation of shear bands is observed in the SEM during the indentation process and is correlated to the appearance of displacement bursts in the load-displacement curve. The effect of varying deformation rates on the formation of shear bands is also investigated.

The second part will show the potential of the same apparatus to perform micropillar-compression experiments on the example of micromachined Si-pillars. It will be shown that by in-situ SEM-observations distinct deformation mechanisms can be seen: the diameter of the pillars has a clear influence on the failure mode and can be correlated to the Weibull distribution of strength.

MM 14.2 Tue 10:45 H16

Scaling in the mechanical properties of thin metal films: from the micro- to the nanoscale — •Ralph Spolenak — ETH Zurich, Zurich, Switzerland

It is well established that the yield stress of thin metal films inversely scales with film thickness as the micron length scale is approached. For thinner films, however, the scaling law changes and also other mechanical properties such as fracture toughness and modulus become affected by the reduced dimensions. Case studies will be presented for thin Cu, Au and Ta films in the thickness range from 10 to 3000 nm on polyimide substrates. Stress-strain curves are obtained by synchrotron based X-ray techniques. The scaling in fracture toughness and yield stress is critically discussed. In addition the effect of temperature on yield stress will be analyzed. In conclusion, thinner is not always better, but an optimal length scale can be found for nanoscale metals.

MM 14.3 Tue 11:15 H16

Direct-Observation Nanomechanical Testing in a Transmission Electron Microscope — •Oden Warren and Ude Hangen — Hysitron, Inc., 10025 Valley View Road, Minneapolis, MN 55344, USA

The intense research interest in nanostructures and nanomaterials has resulted in a strong demand for direct-observation nanomechanical testing. Over the past two years, pioneering quantitative nanoindentation technology for in-situ experimentation in transmission electron microscopes has been developed. This technology has enabled direct investigation of microstructural changes occurring during nanoindentation, as well as direct investigation of the effects of nanocompression on electron-transparent nanostructures such as nanospheres and nanopillars. This presentation will provide examples of deformation mechanisms revealed by the combination of force-displacement curves and corresponding transmission electron microscopy movies. This synergistic combination of high-resolution techniques has led to a fuller appreciation of the fact that mechanical behavior at the true nanoscale is indeed rich and often counterintuitive.

MM 14.4 Tue 11:30 H16

Bulge Testing of Thin Films in an Atomic Force Microscope — •Elmar W. Schweitzer and Mathias Göken — University Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute of General Material Properties, Martensstraße 5, 91058 Erlangen, Germany

Bulge testing of thin membranes is a method, which allows to record stress-strain-curves of thin films without any substrate influence. Pressure is applied to one side of a free standing sample membrane and the deflection as a function of the applied pressure is recorded. Another advantage compared to nanoindentation is a better definition of the stress state in the sample which can be influenced by choosing an appropriate membrane shape.

As soon as the sample dimension reaches the order of magnitude, where physical phenomena, e.g. dislocation motion, come into play, interesting effects can be observed. For example thin metal films show an increase in strength with decreasing film thickness. Furthermore grain boundaries play a more important role, because their volume fraction increases as well.

A self designed bulge test apparatus, which can be incorporated into a Dimension 3100 AFM will be presented. The device can be operated as a standard bulge tester, i.e. pressure-deflection-data of the membrane in question can be recorded. In addition to that, topography images of the loaded membrane surface can be taken to study plasticity effects on a local scale.

MM 14.5 Tue 11:45 H16

Mechanical properties of micro bending-beams: a comparison between discrete dislocation dynamic simulations and experiments — •Christian Motz, Daniel Weygand, and Peter Gumbsch — IZBS, Universität Karlsruhe, D-76133 Karlsruhe

Due to size-effects the mechanical properties in small dimensions may be different from the macroscopic ones and the knowledge of the related mechanisms is essential for a successful design at these small length scales. In complex systems usually stress and strain gradients arises during mechanical loading, and therefore the influence of these gradients on the mechanical properties is important, too. To investigate this influence 3D discrete dislocation dynamic simulations and experiments were performed on micron-sized bending beams. For the simulations the beam thickness varied between 500 nm and 1500 nm with a thickness to length ratio of 1:3. The deformation behaviour was studied in dependence of beam thickness, initial dislocation density and crystal orientation. All configurations showed a pronounced size dependence, i.e. the resistance to plastic deformation increases with decreasing beam thickness, which seems to be mainly caused by a strong dislocation pile-up in the bending beam that is usually not found in the absence of stress gradients (e.g. in compression tests). A comparison with experimental results shows a good agreement in terms of deformation behaviour and possible dislocation structure. A simple analytical pile-up model is developed, which can reproduce the size effect quite well. Finally, the importance of special dislocation structures on the mechanical properties in small dimensions is discussed.

MM 14.6 Tue 12:00 H16

Stress measurments in small dimensions using Confocal Raman Microscopy: a probe for stress and defect density — •Thomas Wermelinger, Cesare Borgia, Christian Solenthaler, and Ralph Spolenak — Lab. for Nanometallurgy, ETH Zurich, 8093 Zürich, Schweiz

Confocal Raman microscopy is a powerful tool for measuring stresses with a lateral resolution in the submicron range in 3D, which as previously only been possible by synchrotron based X-ray techniques. Moreover, it is possible to observe phase transformations, which appear due to high compressive stresses. Residual 3D stress fields in a sapphire single crystals after indentation are analysed. It can be shown that the symmetry of the residual stress field solely depends on the crystal symmetry and not on the symmetry of deformation. A direct correlation between defect structures observed by TEM and the peak broadening in the Raman spectra was found. Raman spectroscopy offers new potential in micro- and nanomechanics.

MM 15: Phase transitions I

Time: Tuesday 10:15–11:15 Location: H4

MM 15.1 Tue 10:15 H4

Combinatorial study of the phase transformation characteristics of Ti-Ni-X (X = Cu, Pd) shape memory thin film composition spreads — •Robert Zarnetta[1,2], Sigurd Thienhaus[1,2], Alan Savan[1], and Alfred Ludwig[1,2] — [1]Combinatorial Material Science group, caesar, Ludwig-Erhard-Allee 2, 53175 Bonn, Germany — [2]Ruhr-University Bochum, Institute of Materials, 44780 Bochum, Germany

The phase transformation properties of Ti-Ni-X (X=Cu,Pd) shape memory thin films prepared in the form of continuous composition spreads were investigated. The thin film materials libraries were fabricated from elemental targets using an ultra-high vacuum combinatorial magnetron sputter-deposition system. Alternating wedge-type layers of Ti, Ni, and Cu (Pd) were deposited on a thermally oxidized Si wafer and subsequently annealed at 500°C for 1h in situ. Automated temperature-dependent resistance measurements (R(T)), energy dispersive X-ray analysis (EDX) and X-ray diffraction measurements (XRD) revealed the compositional region in the ternary phase diagram where thermoelastic transformations occur. The transformation temperatures and the thermal hysteresis were determined from R(T) measurements.

MM 15.2 Tue 10:30 H4

Phonons in High-Pressure structures of Boron — •Jens Kortus[1] and Lilia Boeri[2] — [1]TU Bergakademie Freiberg, Institut for Theoretical Physics, Leipziger Str. 23, 09599 Freiberg, Germany — [2]Max-Planck Institut for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

Boron has recently received a lot of interest in the search of new electron-phonon superconductors. Elemental boron has been shown to undergo a superconducting transition at high pressures. However, no experimental data about the actual crystal structure of the superconducting phase are available. In this work we examine the relative stability of different possible high-pressure phases of boron and calculate the phonon dispersions at the experimental pressures at which superconductivity is observed. The total-energy calculations show that the $\alpha - Ga$ phase of boron, which gives a metal with a low DOS, remains the most energetically favoured one up to very high pressures. Our linear-response results indicate further, that several of the in the literature proposed structures are actually unstable at high pressure.

JK would like to thank the DFG-SPP 1236 for financial support.

MM 15.3 Tue 10:45 H4

Diffuse x-ray scattering from the refractory alloy systems Mo-Ta and Nb-Ta — •Harald Reichert, John Okasinski, Markus Mezger, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

We have performed diffuse x-ray scattering experiments on the bcc refractory alloy systems Mo-Ta and Nb-Ta. Using high energy x-rays in transmission geometry we were able to map the diffuse scattering of single crystalline samples as a function of concentration and temperature. In addition to thermal diffuse scattering we found diffuse scattering from short-range order. Our results will be compared with recently published first-principles calculations [1].

[1] V. Blum, A Zunger, Phys. Rev. B 70, 155108 (2004).

MM 15.4 Tue 11:00 H4

Laser-induced phase transition in As under pressure — •Nils Huntemann, Eeuwe Sieds Zijlstra, and Martin Garcia — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

It has been experimentally shown [U. Häussermann et al., J. Am. Chem. Soc. **124**, 15359 (2002)] that As undergoes a structural transition from the A7 to the simple cubic (SC) structure for increasing pressure. This phase transition occurs in thermodynamical equilibrium. In the last years different nonthermal, ultrafast structural changes have been induced in solids by means of femtosecond laser pulses [A. Cavalleri et al., Phys. Rev. Lett. **87**, 237401 (2001)]. Based on first-principles electronic structure calculations we explored the possibility of inducing nonthermal structural changes in As by ultrashort laser pulses. For this purpose, we determined the potential energy surface (electronic free energy) as a function of the lattice parameters and atomic coordinates for different electronic temperatures, which simulates the ultrafast laser heating of the electrons. Our results indicated that a laser-induced phase transition may occur in As under a pressure of ~ 20 GPa.

MM 16: Phase transitions II

Time: Tuesday 11:45–12:45 Location: H4

MM 16.1 Tue 11:45 H4

Metadynamics Simulations of Phase Transitions in Solids — •Jörg Behler[1], Davide Donadio[1], Roman Martoňák[2], and Michele Parrinello[1] — [1]ETH Zurich, Department of Chemistry and Applied Biosciences, USI Campus, Lugano, Switzerland — [2]Comenius University, Department of Experimental Physics, Bratislava, Slovakia

The theoretical prediction of crystal structures for a given pressure and temperature based only on the chemical composition is still a challenging task. We present a combination of the metadynamics approach, which uses the edges of the simulation cell as collective variables to drive the system away from the local minimum towards a new crystal structure, and an efficient generalized neural network potential representation, which provides the energy and forces as a function of all atomic positions in a system of arbitrary size. This potential is several orders of magnitude faster than the underlying density-functional theory (DFT) calculations while the accuracy of DFT is essentially maintained. The capability of the method is demonstrated for a silicon model system and the results obtained are in excellent agreement with experiment.

MM 16.2 Tue 12:00 H4

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

The early stage of decomposition of supersaturated Cu Fe alloys has been previously intensely studied in the course of classical homogeneous phase separation. Up to now contributions of the strain energy to the decomposition process and its influence on the early stage has been neglected in this system.

In a former study Heinrich et al. (Mat. Sci. Eng. A353 (2003) 92-98) showed that decomposition at low temperatures of supersaturated Cu Co alloys is mainly controlled by strain energy. Hence, cluster's size and morphology are biased and the formation of chains of precipitates in the elastic soft <100> directions of the Cu-matrix is promoted.

In the current study, these phenomena will be investigated for Cu1,7at%Fe after a heat treatment at 722 K for times ranging from 1 to 48 hours. Analyses are performed by utilizing the Tomographic Atom Probe (TAP) and the newly developed computer assisted Field Ion Image Tomography (CFIIT). Amongst others, a chain like formation of precipitates can be observed in our results as well. By means of computer based methodical analyses the directions and distances of alignments of precipitates can be ascertained. The consistency of the results with calculations established by Miyasaki and Yamauchi/ De Fontaine in terms of linear anisotropic elasticity theory will be presented and discussed.

MM 16.3 Tue 12:15 H4

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

Messungen mit Positronen stellen ein wichtiges Hilfsmittel bei der Untersuchung von Gitterfehlern und Ausscheidungen in Metallen dar. Leider lässt sich aus den Messdaten in Form von Positronen-Lebensdauer und Dopplerspektrum der Annihilationsstrahlung nicht direkt auf die Gitterstruktur des Materials schliessen. Durch Simulationsrechnungen für das Positron lassen sich jedoch Lebensdauer und Dopplerspektrum in einem hypothetischen Gitter berechnen. Ein Vergleich der berechneten und gemessenen Werte lässt dann eine Prüfung der Hypothese zu. Auf diese Weise wollen wir die atomare Struktur von Cu-Ausscheidungen in Aluminium im Frühstadium (1-5 Cu Atome) charakterisieren. Die Ausscheidungen wurden mit und ohne Leerstellen mit Hilfe des ab-initio Codes von SIESTA relaxiert.

MM 16.4 Tue 12:30 H4

Simulation of plate shaped second phase particles — •Emmanuel Jannot[1], Volker Mohles[1], Günter Gottstein[1], and Barend Thijsse[2] — [1]Institut für Mtellkunde und Metallphysik, RWTH Aachen, Aachen, Germany — [2]TU Delft, the Netherlands

In several metallurgical systems, plate shaped precipitates are observed. The most well-known example are the GP zones in AlCu alloys, composed of layers of pure copper in the [1 0 0] plane. This morphology is usually attributed to the conjugate effect of a size mismatch between the solute and the matrix atoms and an elastic anisotropy of the fcc lattice, the <1 0 0> direction being the soft and the <1 1 0> the hard direction. The object of this work is to assess the validity of this assertion. For this purpose a MonteCarlo approach is used where the Metropolis algorithm allows finding stable atomic configurations. The configuration energy is evaluated by Molecular Statics. The input parameters of this study are the potentials describing the atomic interactions. At first, harmonic potentials are employed. Using them, a condition for the stability of the plate morphology is found. This result is confirmed using various kinds of pair potentials (Lennard-Jones*). Moreover the Matrix-Solute interaction can be designed to reproduce the precipitate thermal stability. An interfacial energy of 0.08 J/m2 is derived for GP zones in AlCu alloys. Eventually, the influence of dislocations is studied. Simulation results are compared with TEM observations and a mechanism for heterogeneous precipitation in AlCu alloys is proposed.

MM 17: Hydrogen in materials

Time: Tuesday 10:15–11:15 Location: H6

MM 17.1 Tue 10:15 H6

Hydrogen absorption in epitaxial Nb-films: a STM-study — •Kai Nörthemann and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The hydrogen absorption and hydride formation in thin epitaxial films is presented in this contribution, using the model system Niobium-Hydrogen.

With the surface sensitive scanning tunneling microscopy (STM) it is possible to study the hydrogen uptake inside a film because of its strong out-of-plane expansion. Since this is proportional to the H-concentration this effect can, especially, be used to study the hydride evolution. It will be shown that the surface topography tells about the hydride shape and microstructure inside the film. Two different types of hydride-related surface topographies were found: smooth hills (early stages) and rough surface pattern (later stages). The shape of the related hydrides were determined with the help of finite-element analysis. The origin of the two different surface topographies will be presented.

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

MM 17.2 Tue 10:30 H6

The effect of the structure and the stabilizer on the hydrogen absorption in palladium clusters — •M. Suleiman[1], D. Fritsch[2], C. Borchers[1], R. Kirchheim[1], and A. Pundt[1] — [1]1Instiute of Material physics, University of Goettingen Friedrich-Hund-Platz 1, 37077 Goettingen, Germany. — [2]GKSS Research Centre Geesthacht GmbH, Institute of Polymer Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany

In this work the hydrogen absorption behaviour of two types of Pd-clusters, different in structure, will be presented: First, icosahedral Pd clusters stabilized in tetraoctylammonium bromide (TOAB). Second, cubic Pd clusters (Pd-Teflon AF) stabilized in Teflon AF matrix. The phase transition in these samples was monitored by in situ X-ray diffraction. It is shown that the hydrogen uptake ability depends strongly on the lattice structure which is affected by the type of stabilizer. Teflon AF stabilized clusters show the phase transition

which is common for bulk, whereas TOAB stabilized clusters show only weak lattice dilatation upon hydrogen absorption. P-c Isotherms show that the Teflon AF stabilized clusters (the cubic clusters) absorb large amounts of hydrogen both in comparison to bulk Pd and to the TOAB stabilized icosahedral clusters. The measured solubility is higher than that for TOAB-clusters, and even higher than that expected for bulk palladium.. This suggests that surface sites are available for hydrogen in the Pd-Teflon-AF samples which are not accessible for Pd-TOAB-clusters, and that the icosahedral lattice absorbs less hydrogen for similar external pressures.

MM 17.3 Tue 10:45 H6

Temperature dependent FT-IR-spectroscopy on YH_3 — •Stefan Weber and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig

Thin films of yttrium metal have become known under the term of switchable mirrors. Upon hydrogen loading the metallic films undergo a metal to insulator transition, e.g. the opaque metallic films become transparent semiconductors.

Recent Raman studies [1] showed that $YH_{3-\delta}$ behaves like a doped semiconductor which results in an unusual strong temperature dependence of one particular phonon due to electron-phonon interactions. Fourier-transform-infrared-spectroscopy show peaks that can be attributed to hydrogen vibrations by comparison of samples loaded with either hydrogen or deuterium. One of the apparent phonons displays a much stronger temperature dependence than the others. A careful study of the line shapes of deuterium loaded samples reveals a shoulder which can be attributed to an electronic transition between a donor level and the conduction band of $YH_{3-\delta}$. In hydrogen loaded samples this electronic transition coincides with a phonon which hampers its clear identification. But as it doesn't underlay the isotope shift our additional data confirm the assignment of that spectral structure to an electronic transition. This result supports the model of strong correlations in the electronic structure of $YH_{3-\delta}$ [2].

[1] A.-M. Racu and J. Schoenes, Phys. Rev. Lett. 96, 017401 (2006)
[2] K. K. Ng et al., Phys. Rev. B 59, 5398 (1999)

MM 17.4 Tue 11:00 H6

Hydrogen sensors based on magnesium-x (x = Al, Ti, Fe, V and Zn) thin films — •Andreas Laufer, Baker Farangis, Jennifer Stiebich, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

We investigated hydrogen sensors based on magnesium-x (x = Al, Ti, Fe, V and Zn) thin films with a palladium over-layer operating at room temperature. These thin films prepared by RF-sputter-deposition show a very large change in both reflectance and transmittance during the absorption of hydrogen gas. The decrease in reflectance during hydrogenation was studied by using a GaAs infrared emitter and silicon NPN phototransistor as light source and detector. The change of optical properties is believed to result from reversible formation of MgH_x ($x \leq 2$). The reflectance decrease is proportional to the hydrogen concentration (0.1-4% H_2 in Argon). The response time (0-90% of signal) is under 10 seconds depending on the composition of the Mg-alloy.

MM 18: Electronic properties I

Time: Tuesday 11:45–12:45 Location: H6

MM 18.1 Tue 11:45 H6

Energy Loss Magnetic Chiral Dichroism: theory and experiments — •Stefano Rubino[1], Michael Stöger-Pollach[1], Cécile Hébert[1], Peter Schattschneider[1], Jan Rusz[2], and Pavel Novak[2] — [1]Institute for Solid State Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/138, A-1040 Vienna, Austria — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnickà 10, 162 53 Prague 6, Czech Republic

The Transmission Electron Microscope (TEM) has been able to detect Linear Dichroism since many years, yet the possibility to use it to measure circular dichroism as well was only predicted in 2003 and experimentally verified recently with TEM and synchrotron measurements on the same specimen. Angle resolved Electron Energy Loss Spectrometry (EELS) offers several experimental setups able to detect the dichroic signal in the TEM. The choice of the experimental setup influences the achievable spatial resolution as well as the signal to noise ratio. In the experiment, a coherent superposition of two momentum transfer vectors perpendicular to each other is set up, tuning the phase difference between the two interactions to 90°. The inelastic interference term carries the dichroic signature. Experimental details and recent experimental results on Ni, Fe and Co will be presented, as well as simulations. Calculations were done with a full-potential, fully-relativistic Augmented Plane Wave code based on Density Functional Theory. The EMCD technique provides a new analytical tool for the element specific study of local magnetic moments.

MM 18.2 Tue 12:00 H6

Electromigration in Ag(Cu) lines — •R. Emling, U. Schoepka, M. Becherer, and D. Schmitt-Landsiedel — Technical University Munich, Institute for Technical Electronics

Degradation of conducting lines in integrated circuits due to stress by high current density is referred to as electromigration. Voids and hillocks build up by flow of material and increase resistivity until the line breaks or builds a short with an adjacent line. It is well known that small quantities of impurity in a metal can reduce electromigration significantly while resistivity increases only slightly.

In this work thin films of pure Ag and Ag(Cu) with 1.2 % and 2.0 % of Cu were sputter deposited and patterned by a hybrid etching process to produce NIST electromigration test patterns with 5 μm width, 500 μm length and 300 nm thickness. Deposition of the Ag(Cu) alloy was performed by magnetron sputtering using a process newly developed at the institute: Cu wires were attached in parallel to the surface of a pure silver target which resulted in sputtering both, silver and copper, at the same time. The amount of sputtered copper was controlled by the number and thickness of wires. EDX measurements showed a homogeneous dispersion of copper in the layer.

Electromigration measurements were performed at a constant current density of 22 MA/cm^2 until the lines failed within up to 16 days. In this process Ag(Cu) lines with 1.2 % Cu turned out to endure three times longer and lines with 2.0 % Cu up to four times longer than pure Ag lines. In conclusion we can assert a significantly higher electromigration resistance of Ag(Cu) lines.

MM 18.3 Tue 12:15 H6

Pressure effect on the electrical transport and structural properties of TiOCl — •Martin K. Forthaus[1], Timo Taetz[2], Angela Möller[2], and Mohsen M. Abd-Elmeguid[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institut für Anorganische Chemie, Universität zu Köln, Greinstr. 6, 50939 Köln

We have investigated the effect of pressure on the electrical transport and structural properties of the quasi one dimensional Mott insulator TiOCl which exhibits an unconventional spin-Peierls transition at low temperatures. The analysis of the temperature dependence of the electrical resistivity as a function of pressure up to 22 GPa reveals that the energy gap E_g (at 300 K) decreases with increasing pressure with a sudden drop of about 40 % above 12 GPa. However, no metallic state is observed up to 22 GPa. The investigation of the pressure effect on the lattice parameters of TiOCl up to 8 GPa shows an extreme anisotropic decrease with increasing pressure, indicating a structural instability. These results are discussed in terms of a pressure-induced change of the electronic properties which is possibly driven by lattice instabilities under high pressure.

MM 18.4 Tue 12:30 H6

Resistance and magnetoresistance of CuAg alloys — •Jens Freudenberger, Julia Lyubimova, Elias Mohn, Alexandre Gaganov, Nadezda Kozlova, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials

The resistance of cold worked Cu − x wt.-%Ag alloys (x = 7 and x = 24) is measured in dependence of magnetic field and temperature. The influence of impurities (such as vacancies, dislocations, second phases, precipitates, grain boundaries) as well as the size effect on the electrical conductivity of a Cu − 7 wt.-%Ag − 0.05 wt.-%Zr al-

loy wil be discussed. The magnetoresistance (MR) in the field range $0\ \mathrm{T} \leq B \leq 50\ \mathrm{T}$ is positive and increases with magnetic field. Whereas an increase of MR is found for $I \perp B$, no significant change is observed for $I \parallel B$.

MM 19: HV Glatzel

Time: Tuesday 14:00–14:30 Location: H16

Invited Talk MM 19.1 Tue 14:00 H16

Development of Platinum-Based Superalloys by Optimization of Microstructure — •Uwe Glatzel — Metallische Werkstoffe, Universität Bayreuth, Ludwig-Thoma-Straße 36b, 95447 Bayreuth

Development of platinum-based superalloys was carried out by copying the successful system of nickel-base superalloys. The Pt-alloys should have a two-phase microstructure, consisting of a $L1_2$-ordered intermetallic Pt_3Al phase (γ' phase) coherently embedded in a Pt-matrix. Additionally volume fraction, lattice parameter misfit and size of the precipitates have to be optimized. In a first step composition and heat treatment was adjusted to achieve high volume fractions of cuboidal γ' precipitates with a cube size of about 500 nm. Volume fractions of up to 50% could be obtained by ensuring a reasonable temperature window to allow homogenization heat treatment.
By a variation of the Ni-content the misfit between matrix and γ' phase can be adjusted within the desired range of $-3 \cdot 10^{-3}$ up to $-1 \cdot 10^{-3}$. Compression and tension creep tests were carried out. Considering low temperature ductility and testing in air, our optimized alloy results in creep resistance higher than known alloys at a temperature of 1300°C. Additional improvements can be obtained by adding boron in small amounts. Alternatively directional solidified casting would be a promising processing route, which is currently under development.

MM 20: Poster session

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

MM 20.1 Tue 14:45 Poster C

Quantitative Characterization of Thin Film Mechanical Properties using the Bulge-Test-Technique — •Peter Leibenguth and Frank Mücklich — Department for Materials Science, Functional Materials, Saarland University, Saarbrücken, Germany

Because of the limited, if not impossible, applicability of macroscopic characterization methods in the thin film regime, several methods coping with this issue have been developed, e.g. nanoindentation, microtensile-test or substrate-curvature-technique. In contrast to the latter examples, the bulge-test-technique is able to circumvent certain experimental and analytical problems. The underlying principle is quite simple: a geometrically well defined (cirular or rectangular) thin film specimen with simply supported edges is being deflected by a differential pressure acting on one side. By means of exact measurement of the pressure and the resulting displacement, the elastic modulus and the residual stresses of the thin film can be quantitatively investigated in only one experiment. We present the results of our investigations using our new bulge-test-setup, which combines several optimizations to the general technique. Those concern the specimen preparation method, and mainly the exact determination of the deflection, which has been performed using a white-light interferometer allowing a height resolution of approximately 1 nm and a full-field imaging of the specimen geometry. Using nanoindentation, x-ray residual stress analysis and an inverse approach via FEM, the efficiency of this setup was demonstrated inverstigating singlelayered SixNy- and multilayered Al-SixNy- and Cu-SixNy-composite membranes.

MM 20.2 Tue 14:45 Poster C

Enthalpy of Mixing in the Binary System Bi-In — •Andriy Yakymovych[1], Stepan Mudry[1], Christoph Luef[2], and Herbert Ipser[2] — [1]Department of Metal Physics, Ivan Franko National University Lviv, UA-79005 Lviv, Ukraine — [2]Department of Inorganic Chemistry/Materials Chemistry, University of Vienna, A-1090 Vienna, Austria

Bi-In alloys are widely used in manufacturing, for example to make fuel tank safety plugs, or in solders. From the scientific point of view this system is very interesting because of the existence of the intermetallic compounds BiIn, Bi_3In_5 and $BiIn_2$. Transport properties in the liquid state show a deviation of the typical temperature dependence in low temperature regions and knowledge of the thermodynamic properties in the liquid state is very important for deeper understanding of the structure and bonding nature of the system. Most of the investigations of the enthalpy of mixing were made at higher temperatures, the measurement results at lower temperatures, in turn, show some disagreement.

Calorimetric studies of the enthalpy of mixing in the system Bi-In have been carried out at 483, 875 and 1023 K. The enthalpy of mixing is negative and shows a minimum at approximately 45 at.% Bi, what indicates a mutual interaction of both components in the alloys. The curve of enthalpy of mixing is asymmetric.

MM 20.3 Tue 14:45 Poster C

Relaxations in metallic glasses investigated by a broad frequency and temperature range — •Dennis Bedorf[1], Thomas Koeppe[1], Jörg Hachenberg[1], Konrad Samwer[1], Annelen Kahl[2], and Ranko Richert[3] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Keck Laboratories MS 138-78 Caltech, Pasadena CA 91125, USA — [3]Department of Chemistry and Biochemistry, Arizona State University, Tempe AZ 85287-1604, USA

We are interested in glassy dynamics and the atomistic processes leading to different relaxations in amorphous materials. To measure the complex elastic constants, two mechanical spectroscopy techniques were employed. The use of a double-paddle-oscillator (DPO) provides sufficient sensitivity to investigate the loss of even thin films. A DPO is driven in eigenfrequency mode at 5.4 kHz and an amorphous metallic film (PdCuSi) is evaporated onto it and measured under UHV conditions. Cooling and heating enables measurements in a broad temperature range with different heating rates.

To survey the elastic constants at higher frequencies, an ultrasonic spectroscopy technique in the MHz regime is used. The pulse-echo method is applied to a bulk metallic glass in order to obtain the shear modulus and attenuation by monitoring shear wave propagation. The results are discussed in the framework of the Cooperative Shear Model.

This work was supported financially by DFG, SFB 602 and Leibniz Programm.

MM 20.4 Tue 14:45 Poster C

Dynamics in glass forming $Pd_{40}Cu_{40}P_{20}$ melts — •Suresh Mavila Chathoth[1], Bernd Damaschke[1], Michael Marek Koza[2], Ranko Richert[3], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Universitaet Göttingen, 37077 Göttingen, Germany — [2]Institut Laue-Langevin,BP 156 - 38042 Grenoble, France — [3]Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287-1604, U.S.A.

The Cu relaxational dynamics and temperature dependence of self-diffusion in the glass forming $Pd_{40}Cu_{40}P_{20}$ melts has been investigated with inelastic neutron scattering. Unlike in $Pd_{40}Ni_{40}P_{20}$ or $Pd_{43}Ni_{10}Cu_{27}P_{20}$ [1] melts self-diffusion in $Pd_{40}Cu_{40}P_{20}$ melt approaches similar values at high temperature but anomalously faster on approaching its liquidus temperature. The intermediate scattering function, $\Phi(q,t)$ of $Pd_{40}Cu_{40}P_{20}$ melts decay to zero rather non-exponentially. A fitting with Kohlrausch-Williams-Watts function in the α-relaxation regime exhibits structural relaxation that shows stretching in time. Moreover $\Phi(q,t)$ shows temperature and q dependent stretching and is more pronounced at lower temperatures.

This indicates that in the $Pd_{40}Cu_{40}P_{20}$ melts the increase in heterogeneities on cooling towards its liquidus temperature is responsible for the anomalous behavior in the self-diffusivity. We gratefully acknowledge financial support from the Leibniz program.

[1] S. M. Chathoth, A. Meyer, M.M. Koza, F. Juranyi, Appl. Phys. Lett. **85**, 4881 (2004).

MM 20.5 Tue 14:45 Poster C

Dendritic and eutectic solidification of undercooled Ni-Zr alloys — •Helena Hartmann[1,2], Sven Reutzel[1,2], Peter Galenko[2], and Dieter Herlach[2] — [1]Institut für Experimentalphysik IV, Ruhr-Universität, 44780 Bochum, Germany — [2]Institut für Materialphysik im Weltraum, DLR, 51170 Köln, Germany

New measurements of dendritic and eutectic growth velocity in levitated undercooled Ni-Zr samples are performed as a function of undercooling ΔT. The new data reveal high accuracy and low scattering. The growth velocity is measured by using a high-speed camera and subsequently, the morphology of the microstructure of the solidified samples is investigated. The data for eutectic growth of Ni - 8.8 at.% Zr alloy are compared with the previously measured growth velocity data set of dendritic growth of Ni - 1 at.% Zr alloy. Experimental results on kinetics of dendritic and eutectic growth in Ni-Zr alloy samples are discussed and analysed within the current models of non-equilibrium solidification.

MM 20.6 Tue 14:45 Poster C

Interaction of ceramic particles with an advancing dendritic solidification front — •Matthias Kolbe[1], Thomas Lierfeld[1,2], Thomas Schenk[3], Gunther Eggeler[2], and Dieter Herlach[1] — [1]DLR, Institut für Materialphysik im Weltraum, Linder Höhe, 51170 Köln — [2]Ruhr-University Bochum, Institute of Materials IA1, 44780 Bochum — [3]Lab. de Physique des Matériaux, ÉdM de Nancy, France

The interaction of ceramic particles with a dendritic solid/liquid interface has been investigated by undercooling experiments with different levels of convection: (i) in a terrestrial electromagnetic levitation facility (EML) and (ii) in TEMPUS, a facility for containerless processing, under low gravity conditions during parabolic flights. Entrapment of particles in ground experiments and engulfment of a significant fraction of submicron particles under low gravity conditions are attributed to the lower level of convection in the latter experiments and to morphological features of dendritic solidification. X-ray radiography at ESRF has been used for in-situ observations of directional solidification in Al90Cu10 with alumina particles.

MM 20.7 Tue 14:45 Poster C

Depth-resolution measurement of CDB of layered Al-Sn-Sample — •Philip Pikart[1,2], Christoph Hugenschmidt[1,2], Jakob Mayer[1,2], Martin Stadlbauer[1,2], and Klaus Schreckenbach[1,2] — [1]Physikdepartment E21, James-Frank-Straße, 85748 Garching — [2]ZWE FRM-II, Lichtenbergstr. 1, 85748 Garching

At the new positron source NEPOMUC at the FRM-II in Munich a moderated positron beam with an intensity of $\geq 10^8$ positrons per second is available. After linear acceleration up to 30 keV at the entrance of the analysis chamber, coincident doppler broadening (CDB) measurements can be performed.

The implantation depth of the positrons can be varied using different beam energies, and scanning of the positron beam enables lateral resolved analysis of the sample. In this experiment, the minimal visible thickness of the tin-layer is determined by DB measurements and by CDB with improved elemental sensitivity.

For this reason, samples were prepared, which are containing a wedge-shaped layer of tin with a thickness in the range of 1-200nm, on an aluminum substrate and covered by an aluminum layer of constant thickness of $\geq$ 100 nm. The samples were grown out of high purity materials in a MBE-chamber.

The results of the DB-measurements were then compared to CDB-measurements on the same sample with same conditions in order to determine a sensitivity threshold for DB and CDB respectively.

MM 20.8 Tue 14:45 Poster C

Interface Design for adhesion between NiTi shape memory alloy and Polyamide 6 — Stephane Youcheu Kemtchou[1], Guido Grundmeier[2], •Klaus Neuking[1], and Gunther Eggeler[1] — [1]Lehrstuhl Werkstoffwissenschaft, Ruhr-Universität Bochum — [2]Lehrstuhl Technische und Makromolekulare Chemie, Universität Paderborn

Composite Materials consisting of NiTi shape memory alloys as fiber and polymer as matrix have been studied in previous years due to their interesting properties for various applications like vibration control or as actuator. Because of their beneficial properties, especially better adherence to NiTi than thermoplastic polymers, elastomer and thermoset polymers such as epoxy were mostly used as polymer matrix. The aim of the present work was to study different interface systems including organo-functional silane to promote adhesion between NiTi and thermoplastic polymers. A pseudo elastic NiTi alloy and Polyamide 6 as thermoplastic matrix were used for this purpose. The sample was manufactured by injection moulding using in-mould assembly method. Pull- out tests were performed to study the change in adhesion relating to the interface used. The obtained results show significant increase in adhesion related to the interface system used.

MM 20.9 Tue 14:45 Poster C

Formation of rare earth zirconia pyrochlores on yttria-stabilized ZrO_2 single crystals by solid state reactions — •Andreas Schubert, Stephan Senz, and Dietrich Hesse — Max Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

$RE_2Zr_2O_7$ (RE=La, Pr, Nd, Sm, Gd, Ho)-based pyrochlore islands were grown on Y_2O_3-stabilized ZrO_2 (YSZ) single-crystals by reaction between RE_2O_3 and YSZ. After a vapour-solid reaction at 1200 °C at a rate of 0.6 nm/min for 6.5 min between La_2O_3 vapour and YSZ(001), islands with eight domains were formed. Four domains were tilted by 2.1° around <110> and the other four were tilted by 0.9° around <100>. To understand this effect, other experiments were performed with different substrate orientations and other rare earth oxides, to study the influence of the misfit. $La_2Zr_2O_7$ (LZO) has a relatively large misfit to YSZ of 5 % but other rare earth-based pyrochlores have lower misfits of 4.0 % ($Pr_2Zr_2O_7$) to 1.2 % ($Ho_2Zr_2O_7$). The reaction products were investigated by AFM, XRD and TEM. On YSZ(110), four domains were found by XRD pole figure measurements, two were tilted around $[1\bar{1}0]$ with a maximum at a tilt angle of 0.6° and the other two were tilted by 0.9° around [001]. AFM and TEM plan-view images show stripe-shaped islands with the long edge along $[1\bar{1}0]$ and the short edge along [001]. In addition to these vapour-solid reactions some experiments with solid-solid reactions were performed. For the solid-solid reaction of La_2O_3 and YSZ(001) it was determined by XRD-measurements that the relation (001)LZO ∥ (001)YSZ is valid without any systematic tilt (FWHM=0.5°).

MM 20.10 Tue 14:45 Poster C

Removing relativistic effects for the determination of optical properties using EELS — •Michael Stöger-Pollach, Anita Laister, and Peter Schattschneider — Institute for Solid State Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/138, A-1040 Vienna, Austria

Since the energy resolution of modern energy loss (EELS) experiments in a transmission electron microscope (TEM) has improved to less than 0.2 eV full width at half maximum in the elastic peak, valence EELS has attracted interest again. However, due to the fact that the acceleration voltages of conventional TEMs are in the range of 100-300 kV retardation effects become important. The condition for Cerenkov radiation is fulfilled if v > c/n, with c as the speed of light, v as the speed of the probe electron and n as the refractive index of the material.

For determination of optical properties Kramers-Kronig Analysis (KKA) is applied after an iterative removal of relativistic effects and surfce plasmons. Conventinal software does not take relativistic effects into account. Our method therefore gives more precise information on the optical properties of materials. Moreover faint differences of the response function between similar layers can be probed with very high accuracy.

We present the result on two similar SiN:H layers with different H concentration. The difference in the optical refractive index is 2% and can be identified with an accuracy of less than 1%.

MM 20.11 Tue 14:45 Poster C

ELNES at Internal Copper-Silicon Dioxide Interfaces — •Oliver Heckl[1], Ferdinand Haider[1], and Jürgen Gegner[2] — [1]Universität Augsburg, Institut für Physik, Lehrstuhl für Experimentalphysik I, Physik Geb. Nord, Ebene 3, Universitätsstr. 1, D-86159 Augsburg — [2]SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany, E-mail: juergen.gegner@skf.com

Metal-silicon dioxide interfaces are of special importance in semiconductor technologies (e.g. MOS structures). A Cu-Si alloy containing

1.5 at.% Si is produced by arc melting. Samples of 200μm in thickness are completely internally oxidized in a Rhines pack powder mixture at 1000°C. Spherical amorphous SiO_2 precipitations are formed homogeneously dispersed within the copper matrix.

The heterophase boundary between the base metal and the embedded oxide particles is examined with high spatial resolution using a scanning transmission electron microscope (STEM) that is equipped with an electron energy loss (EEL) spectrometer. Typical features of the electron energy loss near-edge fine structure (ELNES) of the oxygen O-K ionization edge allow to determine the bonding state of oxygen and thus to detect interlayers at the phase boundary. The validity of the Kirchheim structural vacancy model of oxygen segregation at metal-oxide interfaces shall be verified this way: for amorphous precipitations, it predicts that no interfacial accumulation of excess oxygen atoms should occur.

MM 20.12 Tue 14:45 Poster C

SIMS and XRD Measurements for the Critical Review of Carbon Diffusivity Derivation from Hardness Profiles — •Jürgen Gegner — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Microhardness decarburization profiles are often used in the industry to estimate the carbon distribution in steels. For quantitative evaluation, an analysis based on diffusion theory must be performed, the fundamentals and mathematical basics of which are presented. If the relationship between hardness and carbon content is known, microhardness-distance curves of steels can be analyzed in this way. For martensitic grades, for instance, a linearized expression holds in the concentration range from 0.15 to 0.6 m.% C. Microhardness depth profiles of higher carbon steels and other microstructures, however, are also evaluated in the literature. The applicability of quantitative diffusion modeling is discussed in detail. Through hardenable rolling bearing steel 100Cr6 (1.3505, SAE 52100) serves as model material: carbon concentration-distance curves are measured with high accuracy by secondary ion mass spectrometry (SIMS) and compared with microhardness decarburization profiles for tempered and untempered martensitic and near-equilibrium microstructures, which are further characterized by metallographic micrographs. Also, the correlation to X-ray diffraction (XRD) characteristics is considered.

MM 20.13 Tue 14:45 Poster C

Experimental and Theoretical Analysis of Fatigue Phenomena in Rolling Contact — •Jürgen Gegner and Wolfgang Nierlich — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Material mechanics theories of rolling contact loading can be reassessed by recording the alteration of X-ray diffraction (XRD) characteristics measured from the edge to the core. Exceeding metallographic investigations, the developments of residual stresses and XRD line width represent the relevant information carrier. Material changing permits a specific correlation to failure probability distributions. These relationships differ significantly for sub- and near-surface fatigue. Recent findings from demanding bearing applications point to different equivalent stresses for describing the material response in both loading types: for classical sub-surface rolling contact fatigue (RCF) that is characterized by strengthening and softening processes below the Hertzian contact area, shear stress-based hypotheses are indicated, whereas for the surface failure mode that is accompanied by embrittlement, the main normal stress-based hypothesis should additionally be considered. Cyclic tensile stresses caused by friction can act on material-inherent crack sources. In both cases, line width changes, which mainly stem from plastic deformation with rearrangement of the dislocation configuration and martensite decay with carbon diffusion, serve as powerful sensor for material aging. Rig tests under controlled mixed friction conditions give an example of near-surface RCF.

MM 20.14 Tue 14:45 Poster C

Miniaturisation of the shear compression specimen — •Markus Ames, Jürgen Markmann, and Rainer Birringer — Universität des Saarlandes, Saarbrücken, Deutschland

The shear compression specimen has been developed for large strain testing of materials. It consists of a short cylinder or cuboid with two slots oriented at 45° relatively to the longitudinal axis (gauge section). As a result of this geometry, uniaxial compression leads to a predominant shear deformation localized across/along the gauge section. The obtained data has been evaluated by comparing the experimental data with finite element simulations of the deformation process, using material properties like young modulus and yield stress as input parameters.

The purpose of the present study was to explore the potential for miniaturising this specimen geometry in order to become applicable for mechanical testing of small-sized nanostructured materials. Therefore, the geometry of the conventional shear compression specimen (a cylinder of 20mm height and 12.65mm in diameter) has been stepwise affinely shrunk to cuboids of 7 x 3.6 x 0.5mm in size. We used the spark erosion technique to prepare specimen of OFHC copper, and we will discuss, based on yield stress and modulus, under which conditions the mechanical behaviour of such miniaturised specimen appears shape and size invariant.

MM 20.15 Tue 14:45 Poster C

Calculation of the *Peierls stress* from atomistic simulations for bcc tungsten: screw vs. edge dislocations — •Bernd Eberhard[1,2], Juergen Almanstoetter[2], and Ferdinand Haider[1] — [1]Universität Augsburg, Institut für Physik — [2]OSRAM GmbH, Mittelstetter Weg 2, 86830 Schwabmünchen

For bcc metals, it is commonly assumed, that the mobility of screw dislocations is significantly lower than that of edge dislocations and, therefore, should control the low temperature plastic deformation behaviour. The mobility of dislocations depends on their *Peierls energy barrier*, defined as the activation energy required to move a dislocation in an otherwise perfect crystal. This connection between atomistic features and the overall mechanical behaviour makes a more detailed investigation of the atomistic system necessary. Also, the violation of *Schmid's Law*, stating that the critical resolved shear stress is constant and independent of the slip system and the external stress, is an important ingredient for the construction of macroscopic flow rules of the material, suitable e.g. for *finite element* calculations.
In present work, these effects are studied for $1/2a\,\langle 111\rangle$ *screw* and *edge* dislocations in tungsten.
To this end, we constructed dislocation dipoles using elasticity theory in a periodic simulation cell. After relaxation within a NPT MD-simulation, we applied an external shear stress to the system in order to force the dislocations to move at low simulation temperatures. The *Peierls energy barriers* and the corresponding *Peierls stresses* are derived.

MM 20.16 Tue 14:45 Poster C

Analytical and numerical evaluation of the critical tensile stress for failure event in single-crystal sapphire detected by the combined application of normal and lateral forces — •Maksim Karniychuk[1], Vladimir Kolchuzhin[2], and Frank Richter[1] — [1]Technische Universität Chemnitz, Institut für Physik, 09107 Chemnitz — [2]Technische Universität Chemnitz, Fakultät für Elektrotechnik und Informationstechnik, 09107 Chemnitz

The new possibilities for mechanical characterization of bulk and coated materials by the combined application of normal (UMIS 2000, CSIRO) and lateral (LFU, ASMEC) forces were recently developed [1,2]. Among others, the possibility for experimental detection of crack formation was offered. As an example, the crack formation was detected in single-crystal sapphire from the shape of the lateral force-displacement curves at a given normal force. Thus, the value of critical tensile stress for crack formation in material can be evaluated by both analytical and numerical approaches at the known critical normal and lateral forces.

The presented work reports results of comparison of critical tensile stress evaluations performed by both mentioned approaches. The analytical approach uses the Hanson model for bulk materials realized by the software Elastica (ASMEC). Finite Element Method is used for numerical evaluation by means of the commercial software ANSYS.

[1] V. Linss, T. Chudoba, M. Karniychuk, F. Richter, Thin Solid Films 494 (2006) 179

[2] M. Karniychuk, Ph.D. thesis, TU Chemnitz, 2006

MM 20.17 Tue 14:45 Poster C

Martensite formation in a ductile Cu47.5Zr47.5Al5 bulk metallic glass composite — •Simon Pauly, Jayanta Das, Cécilie Duhamel, and Jürgen Eckert — IFW Dresden, Postfach 27 01 16, D-01171 Dresden

A Cu47.5Zr47.5Al5 alloy was solidified into rods of 2, 3 and 5 mm diameter and the microstructures as well as the elastic and plastic properties were investigated along the length of each rod. It was found that neither the microstructure nor the mechanical properties vary significantly along the length of the specimens, except for the 5 mm diameter rod where the top part was proved to be fully crystalline containing

cubic B2 CuZr (austenite) and monoclinic CuZr (martensite) phases. A composite microstructure consisting of B2 CuZr embedded in an amorphous phase was revealed in the other parts of the 5 mm diameter and along the 2 mm and 3 mm diameter rods. The differently solidified alloys show high strength (σy up to 1721 MPa) and a distinct deformability (ϵp up to 10.1 %) under uniaxial compression and a work hardening-like behavior.

MM 20.18 Tue 14:45 Poster C

In-situ Observation of Phase Formation in Undercooled Nd-Fe-B-melts with Synchrotron Radiation and High-Speed Video Analysis — •Jörn Strohmenger[1,2], Thomas Volkmann[2], Jianrong Gao[3], Sven Reutzel[1,2], Dirk Holland-Moritz[1], Oliver Heinen[1], and Dieter Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum f. Luft u. Raumfahrt, 51170 Köln — [2]Institut für Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum — [3]Key Lab of Electromagnetic Processing of Materials, Northeastern University Shenyang, 110004, P.R. China

Competitive crystallisation of stable and metastable phases in undercooled Nd-Fe-B melts was investigated using electromagnetic levitation technique combined with in-situ X-ray diffraction experiments at the ESRF. It is shown that the primary crystallizing phase is influenced by undercooling, e.g a metastable phase can be directly observed which initiates the formation of the intermetallic Phi-phase. It can be identified as a ternary extension of the rhombohedral Nd2Fe17 phase being stable in binary Nd-Fe alloys. The growth velocity of Phi-phase is determined with a high-speed camera sytem.It is shown that growth velocity is affected by induced melt convection. A phase selection diagram showing the different solidification pathways as a function of undercooling and alloy composition will be analyzed within theories of nucleation and crystal growth. This work was supported by DFG under contract No. HE1601/14.

MM 20.19 Tue 14:45 Poster C

USAXS measurements of short- range ordering in mesoscopic systems — •Ina Klassen[1], Patrick Wette[1], Dieter Herlach[1], Dirk Holland-Moritz[1], and Stephan Roth[2] — [1]Institute of Materials Physics in Space, 51147 Cologne, Germany — [2]Hasylab at Desy, 22603 Hamburg, Germany

High resolution ultra- small x- ray scattering techniques at Hasylab are used to determine the fluide and crystalline structure factor of charged colloidal suspensions. We analyse charged stabilised silica particles of 200nm radius with different volume fractions and salt concentrations. By varying the salt concentration we tune the electrical potential which influences the structural behavior of colloidal crystals. In addition to x-ray scattering we show light scattering experiments and compare the experimental results of both techniques with respect to structural information.

MM 20.20 Tue 14:45 Poster C

Primary crystallization of the hypoeutectic Ni-17at% P alloy by ASAXS and SANS — Dragomir Tatchev[1], •Rainer Kranold[2], Armin Hoell[3], Günter Goerigk[4], and Stephan Armyanov[1] — [1]Institute of Physical Chemistry, BAS, Sofia 1113 — [2]Institute of Physics, Rostock University, Rostock — [3]Hahn Meitner Institute, Glienicker Str. 100, Berlin — [4]Institute of Solid State Research, Jülich Research Centre, P.O. Box 1913, Jülich

We investigated the primary crystallization of Ni(P) particles in the amorphous hypoeutectic Ni-17 at.% P alloy with anomalous small-angle X-ray scattering (ASAXS) [1] and small-angle scattering of polarized neutrons (SANS) [2]. Using the maximum entropy method, the particle size distribution, the size dependence of the particle composition and the amorphous matrix composition were determined simultaneously. The size distribution shows a peak at particle radius of 1 nm and a tail spanning from 2 to 15 nm. The composition of the particles of the peak changes from 14 to 2 at.% P as their radius grows from 0.7 to about 3 nm. The particles in the tail of the size distribution (2-15 nm) have nearly constant P content in the range of 0-2 at.%. The matrix composition tends to the eutectic composition with 19 at.% P at the end of the primary crystallization process. It should be mentioned that our experimental results completely confirm the predictions made in a generalized Gibbs' approach to nucleation theory [3] developed recently. [1]D. Tatchev et al., J. Appl. Cryst. 38 (2005) 787. [2]D. Tatchev et al., Physica B 369 (2005) 8. [3]J.W.P. Schmelzer et al., J. Colloid Interface Sci. 272 (2004) 109.

MM 20.21 Tue 14:45 Poster C

Modeling of dendritic solidification *in undercooled dilute Ni-Zr melts — Denis Danilov[1], Peter Galenko[2], •Britta Nestler[1], and Dieter Herlach[2] — [1]Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany — [2]Institut für Raumsimulation, DLR, Köln

The dendritic and eutectic solidification in undercooled Ni-Zr samples is analyzed using new experimental results, theoretical studies based on a sharp-interface model and phase-field simulations. Predictions of a sharp interface model and of a diffuse interface model describing the phase transition under the consideration of both, thermal and solutal diffusion are compared with the experimental results evaluating the dendritic tip velocity in electromagnetically levitated Ni-Zr samples.

MM 20.22 Tue 14:45 Poster C

Phase-field modelling of solute trapping during rapid solidification of a Si–As alloy — Denis Danilov and •Britta Nestler — Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany

The effect of nonequilibrium solute trapping by a growing solid under rapid solidification conditions is studied using a phase-field model. Considering a continuous steady-state concentration profile across the diffuse solid-liquid interface, a new definition of the nonequilibrium partition coefficient in the phase-field context is introduced. This definition leads, in particular for high growth velocities, to a better description of the available experimental data in comparison with other diffuse interface and sharp-interface predictions.

MM 20.23 Tue 14:45 Poster C

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

We developped a real space technique which includes local atomic relaxation after each MC step, allowing thus to study phase transformations 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.

This method was used to study segregation to an edge dislocation. The pinning force was calculated by shifting the concentration profile and subsequent relaxation of the lattice. Furthermore the method was applied to calculate the phase diagram using an EAM potential. This was done using grand canonical simulations at different temperatures and chemical potentials.

MM 20.24 Tue 14:45 Poster C

Nucleation kinetics in deionized charged colloidal model systems: a quantitative study by means of classical nucleation theory — •Patrick Wette[1] and Hans Joachim Schöpe[2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln — [2]Institut für Physik, Johannes Gutenberg Universität , Staudinger Weg 7, 55128 Mainz

We have studied the nucleation kinetics of charged colloidal model systems under salt free conditions covering a wide range of particle number densities $18\mu m^{-3} \leq n \leq 66\mu m^{-3}$.We employed direct video-microscopic observation of individual nucleation events to obtain time resolved nucleation rate densities. Polarization microscopy and static light scattering on the resulting solids in combination with Avrami-theory is used to determine the steady state nucleation rate at high undercoolings. The final nucleation rate densities J from different methods are observed to be consistent with each other. By increasing the difference in the chemical potential between melt and crystal $\Delta\mu$ about one order of magnitude J increases over eight orders of magnitude. The data can be well analyzed and interpreted using classical nucleation theory (CNT) leading to a linearly increasing melt/crystal surface tension. Surprisingly the reduced surface tension is about one order of magnitude larger compared to other system (metals, hard sphere colloids). The critical radius of the crystal nuclei is decreasing down to a very small value of 1.5 coordination shells. The determined kinetic prefactors are up to 15 orders of magnitude smaller than the prefactor calculated by CNT.

MM 20.25 Tue 14:45 Poster C

Analytical bond order potential for bcc and fcc iron - comparison with established EAM potentials — •Michael Müller,

Paul Erhart, and Karsten Albe — TU Darmstadt. Institut für Materialwissenschaft, FG Materialmodellierung, Petersenstr. 23, D-64287 Darmstadt

A new analytic bond-order potential for iron is presented that has been fitted to experimental data and results from first-principles calculations. The angular dependent functional form allows a proper description of a large variety of bulk, surface and defect properties, including the Bain-path, phonon dispersions, defect diffusivities and defect formation energies. By calculating Gibbs free energies of bcc and fcc iron as a function of temperature, we show that this potential is able to reproduce the transitions from alpha-iron to gamma- and delta-iron before the melting point. The results are compared to four widely used embedded atom method potentials for iron.

MM 20.26 Tue 14:45 Poster C

Sample preparation from mechanically alloyed CuFe powders by means of focussed ion beam — •Malte Schmidt, Talaat Al-Kassab, Catharina Wille, and Reiner Kirchheim — Georg-August-Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

The focussed ion beam (FIB) has been utilised to shape tip samples for field ion micrsocopy (FIM) and tomographic atom probe (TAP). These tips were prepared from powder particles of $Cu_{97.5}Fe_{2.5}$, $Cu_{95}Fe_5$ and $Cu_{90}Fe_{10}$. Such powder particles are first produced using a high-energy planetary ball mill under protective Ar atmosphere, using elemental powders of high purity and milling tools made of hardened steel. Subsequently the milled powder was dusted onto a double-stick carbon tape adhered to a FIB-specimen holder.

A modified lift-out method, which is usually used to fabricate transmission electron microscope lamellae, is applied as a first step of the procedure. After cutting out the lamella of a single particle of the powder, a longish cuboid with an approximate 2μm x 2μm base area is lifted out of the particle and immediately welded onto a modified tungsten tip by means of platinum ion assisted deposition. Subsequently the actual FIM - tip can be shaped out of this cuboid. In this contribution the different steps of the novel procedure are explained and discussed in detail emphasising the sharpening techniques. In addition first results of measurements of such prepared samples will be presented.

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

MM 20.27 Tue 14:45 Poster C

Sintering without grain growth? A strategy for compacting nanostructured powders to high density without loss of nanocrystallinity — •Lionel Kroner and Carl Krill — Institute of Micro and Nanomaterials, Ulm University, D-89081 Ulm

Most synthesis routes for nanocrystalline materials result in thin films or powders, which can in principle be formed into bulk specimens via compaction. However, achieving near-100% density generally requires the simultaneous application of high temperature, which in turn induces grain growth, and the final product is no longer nanocrystalline! A potential strategy for sintering without significant grain growth would be to suppress the driving force for coarsening through the deliberate addition of an atomic species that segregates to the grain boundaries. Such *thermodynamic stabilization* of nanocrystallinity has already been demonstrated for ball-milled Pd doped with Zr [1]; however, no attempt was made to compact the resulting powders into bulk specimens. In this work, we examine the grain size and porosity of nanocrystalline $Ni_{1-x}Zr_x$ powders as a function of Zr concentration and temperature, both under atmospheric pressure and after compaction. The microstructural evolution during pressureless annealing is followed nondestructively using high-temperature wide-angle x-ray diffraction, and the density of compacted powders is determined by Archimedes' method. The influence of Zr addition on the sinterability of the powders is assessed.

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

MM 20.28 Tue 14:45 Poster C

Reactive interdiffusion in sandwich type Al/Cu thin-films — •Constantin Buzau Ene[1], Carsten Nowak[1], Guido Schmitz[2], Talaat Al-Kassab[1], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Friedrich-Hund Platz 1, D-37077, Göttingen, Germany — [2]Institut für Materialphysik, Wilhelm-Klemm-Str.10, D-48149 Münster, Germany

Al/Cu/Al and Cu/Al/Cu triple layers with approximately 10nm single layer thickness deposited on tungsten substrates and planar (100) Si were analyzed in the early stages of reactive interdiffusion by atom probe tomography and TEM. The first reaction product is found after 5 min at 110°C and identified with a composition around the Al_2Cu. Surprisingly, we found a significant asymmetry in the reaction rate with the stacking sequence as a particularity of the tip-shaped tungsten tips: The thickness of the product grown at the interfaces Cu grown on Al layer, is approximately 1.5 to 2 times thicker than at the other interfaces at which Al grows on a Cu layer. Compared to the recently proven delayed nucleation of the first product phase in the case of Al/Co thin-films, which has been explained by the concept of a critical gradient, the reaction in Al/Cu develops quite differently. Applying the critical gradient concept to the Al/Cu system leads to the prediction of a critical nucleation thickness of 6.8 nm. This is in obvious contrast to the experiment, which reveal parabolic growth from the very beginning with no precursory interdiffusion and no distinct nucleation process. Thus,in the case of Al/Cu the first reaction product might be a metastable one. Pasichnyy et al, Phys. Rev. B 72 (2005).

MM 20.29 Tue 14:45 Poster C

Nanolayered and nanoparticle-dispersed WC/C coatings: frictional and wear behavior — Maik Gubisch[1], •Yonghe Liu[2], Sven-Erik Wulf[1], Thomas Haensel[2], Mikhail Kosinskiy[2], Lothar Spiess[1], and Juergen A. Schaefer[2] — [1]Institut für Werkstofftechnik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany — [2]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

The control of friction plays a critical role in the developing of wide scanning-range nanopositioning technology, which usually employs bearings to cover the wide distance. A series of WC/C coatings have been developed for the application on the bearings. They are processed in two kinds of microstructures: nanoscale multilayer of WC and amorphous carbon, and nanoscale crystalline WC particles in an amorphous carbon matrix. In this work, we compared their frictional and wear behaviour measured by a microtribometer, and correlated with the microstructure of the worn tracks and transfer films characterized by SEM, EDS, FIB and TEM. Though the frictional behaviour seems quite similar, the wear resistance of the coatings is quite different. These findings are discussed with the formation and redistribution of the transfer films.

MM 20.30 Tue 14:45 Poster C

Boron Sheets and Boron Nanotubes — •Jens Kunstmann[1] and Alexander Quandt[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Institut für Physik der Universität Greifswald, Domstraße 10a, 17489 Greifswald

Based on a numerical ab initio study, we discuss a structure model for a broad boron sheet, which is the analog of a single graphite sheet, and the precursor of boron nanotubes. The sheet has linear chains of sp hybridized sigma bonds lying only along its armchair direction, a high stiffness, and anisotropic bonds properties. The puckering of the sheet is explained as a mechanism to stabilize the sp sigma bonds. The anisotropic bond properties of the boron sheet lead to a two-dimensional reference lattice structure, which is rectangular rather than triangular. As a consequence the chiral angles of related boron nanotubes range from 0 to 90 degrees. Given the electronic properties of the boron sheets, we demonstrate that all of the related boron nanotubes are metallic, irrespective of their radius and chiral angle, and we also postulate the existence of helical currents in ideal chiral nanotubes. Furthermore, we show that the strain energy of boron nanotubes will depend on their radii, as well as on their chiral angles. This is a rather unique property among nanotubular systems, and it could be the basis of a different type of structure control within nanotechnology.

MM 20.31 Tue 14:45 Poster C

Influence of bonding on the I-V-characteristics of Si29H24 and organic molecules on Si surfaces — •Samuel Baltazar-Rojas[1,4], Daungruthai Jarukanont[1], Mario De Menech[1,2], Ulf Saalmann[2], Aldo Romero[3], and Martin Garcia[1] — [1]Theoretische Physik, FB 18, Universität Kassel, Kassel, Germany — [2]Max–Planck–Institut für Physik komplexer Systeme, Dresden, Germany — [3]CINVESTAV, Queretaro, Mexico — [4]Advanced Materials Department, IPICYT, San Luis Potosi, Mexico

In the last years, much attention has been given to the study of trans-

port properties through supported clusters and molecules, and it has become more intensive in the last years due to the different potential applications of these systems to electronic devices. We present a theoretical study of charge transport through clusters and molecules supported on silicon surfaces. The method simulates the measurement of the I-V characteristics with the help of a STM tip. The electronic properties of the cluster (molecule) coupled to the surface and the STM are calculated using non-equilibrium Green's functions based on effective single-particle Hamiltonians. In particular, we have computed conductance spectra of H-passivated silicon cluster $Si_{29}H_{24}$ on an ideal Si surface, showing the importance of the surface to modulate and control the I-V curve. Also, we have considered organic molecules such as styrene and show that negative differential resistance can appear due to the shifting of the electronic levels near bulk of the Si substrate with the external bias. We analyze the effect for different configurations of the supported organic molecule.

MM 20.32 Tue 14:45 Poster C

Microstructure in Damascus Sabres — •Marianne Reibold[1], Peter Paufler[1], Dirk Meyer[1], Alexander Levin[1], and Werner Kochmann[2] — [1]Institut für Strukturphysik, TU Dresden, D-01062 Dresden, Germany — [2]Krüllsstrasse 4b, D-06766 Wolfen

Damascus steel is famous for its beauty and excellent mechanical properties. Damascus blades - originating in India - were manufactured from so-called "wootz" steel.

For a better understanding of the ancient technology by analysis of the microstructure of damascene steel, high-resolution electron microscopy (TEM) and X-ray diffraction are eligible tools. The specimens investigated were taken from a genuine Damascus sabre produced by the blacksmith Assad Ullah in the seventeenth century.

The main results are as follows: Besides ferrite and perlitic cementite, we observed a third form of cementite forming so-called nanowires. These nanowires often arrange in colonies. Preferably, the {010}-lattice planes of the nanowires are oriented along the longitudinal direction. The surrounding of the nanowires often could be idendified as alpha-ferrite.

After dissolution of the sample in hydrochloric acid, carbon-nanotubes became visible. Some remnants showed evidence of incompletely dissolved cementite nanowires, indicating that these wires could have been encapsulated and protected by the carbon nanotubes. [1]

[1] Reibold et al., Nature 444,(2006) 286.

MM 20.33 Tue 14:45 Poster C

Development of an EAM potential for ruthenium — •Frank Römer and Thomas Kraska — Physical Chemistry, University Cologne, Luxemburger Str. 116, D-50939 Köln

The embedded atom method (EAM) is an effective potential model for metals that consists of a functional of the local electron density, being a multibody interaction, and a pairwise additive repulsion potential for the atomic cores. In the context of the development of an EAM potential for the hcp metal ruthenium different concepts are investigated in detail. The ability to reproduce mechanical and caloric properties are analysed for various methods generating the different terms of the potential. Instead of fitting to experimental data, a new analytical expression for the screening function or the effective core charge, based on the electron distribution, is proposed. Because of the lack of knowledge about the effective electron configuration of ruthenium, which is also the case for several other transition metals, the influence of given electron configurations and the resulting electron distribution function on the physical properties is investigated. The properties included here are the stable structure, the lattice constants, and the cohesive energy. In this way the electron configuration can be determined from the associated preferred bulk structure. Vice versa the correlation between the devolution of the electron density and the difference in energetic stability of the two close-packing of spheres, hcp and fcc, are investigated.

MM 20.34 Tue 14:45 Poster C

Spatiotemporal stroboscopic interferometry on nanomechanical resonators — •Fabian Giesen[1,2], Miroslav Belov[3], Joseph Losby[1], Jennifer Moroz[1], Alastair Frasier[1], Graham McKinnon[3], Yuebin Ning[3], and Mark R. Freeman[3,4] — [1]Department of Physics, University of Alberta, Edmonton, Canada T6G 2G7 — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Str. 2A, 12489 Berlin — [3]Norcada Inc., 4465 - 99 street, Edmonton, Canada T6E 5B6 — [4]National Institute for Nanotechnology, Edmonton, Canada T6G 2M9

Despite the fundamental and application oriented interest of nanomechanical structures, the detection of their motion remains a challenge. We present spatiotemporal interferometric detection of the motion of microstructured cantilevers and doubly-clamped beams. This technique is capable of broadband detection with picosecond time resolution and micrometre spatial resolution. The actuation is achieved through fast voltage pulses triggered by a pump laser pulse. The subsequent motion is detected through the interferometric contrast of a probe laser spot reflected from the vibrating structure and the sustrate. We discuss the calibration of the interferometric contrast to obtain absolute values of the vibration of our silicon based nanostructures. We also demonstrate the capability of imaging the out-of-plane flexural modes of our cantilevers. Our work was supported by iCore, CIAR, and NSERC

MM 20.35 Tue 14:45 Poster C

Aspects of the electrical resistance of hydrogen loaded Pd thin films — •Stefan Wagner and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37073 Göttingen

While the knowledge on the electrical resistance response of bulk Pd due to hydrogen loading is well established in literature, little is known on the response of Pd thin films. In the present contribution first results of systematic studies on sputtered Pd films in the thickness range from 10 to 200 nm will be presented. Hysteretic effects and hydrogen-content dependent response times of the resistance propagation have been observed, that will be discussed in terms of kinetic and structural aspects of the Pd-H system. The electrical resistance turns out to be an easily operated measure for the determination of the phase boundaries of the Pd-H system.

MM 20.36 Tue 14:45 Poster C

Hydrogen in epitaxial V-8at%Fe films on Al2O3 substrate — •Ryota Gemma, Talaat Al-Kassab, Reiner Kirchheim, and Astrid Pudnt — Institut fuer Materialphysik, Goettingen, Germany

In this study, P-C-T properties and hydrogen-induced stresses of V-8at%Fe 100nm thick films with different microstructures and different initial strain conditions were investigated by measuring electromotive force (EMF) and in-plane stress simultaneously. The phase boundaries for the solid solution cH,α and the hydride cH,β were determined. The local chemistry of the hydride (deuteride) was investigated by performing tomographic atom probe analysis (TAP). The phase boundaries were found to be microstructure dependent: The α-phase solubility limit cH,α=0.1 H/V and cH,β= 0.45 H/V for films with small domain size, and cH, α=0.1 H/V and cH,β= 0.6 H/V for films with large domain size. The total in-plane compressive stress was smaller in small-domain samples compared to larger-domain samples. It was shown that the measured slope of P-C isotherm depends on initial stress condition and the microstructure. TAP analysis at 22K detected a plate-like deuteride VD0.65 at Pd/V interface. The concentration of this precipitate was in accordance with the expectations.

MM 20.37 Tue 14:45 Poster C

Preparation and optical characterisation of rare earth hydride films — •Helge Schröter, Stefan Weber, and Joachim Schoenes — Inst. für Physik der Kondensierten Materie, Medelssohnstraße 3 38106 Braunschweig, Germany

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 (YH2) and finally to a transparent insulator (YH3). Europium also undergoes a metal to insulator transition, in contrast to yttrium-hydride it additionally undergoes a transition from antiferromagnetism to ferromagnetism. For an understanding of the mechanism driving this metal-insulator transition, the precise measurement of the optical properties is mandatory. Therefore the change of the optical properties of the samples connected with the metal insulator transition, was examined by spectroscopic ellipsometry which allows a direct measurement of the dielectric function. Because of the reactivity of the pure rare earth metals it is difficult to grow stable films. We have used two methods to prepare hydride-films: (I) growth of in-situ hydrogenated films by pulsed laser deposition in a hydrogen atmosphere. By variation of the hydrogen pressure thereby, it is possible to grow layers with different hydrogen concentrations. (II) growth of pure rare earth metal films by molecular beam epitaxy and subsequent evaporation of a protective Pd cap-layer . These films have been hydrogenated ex-situ in an hydrogen-cell which is directly inserted into

the ellipsometer.

MM 20.38 Tue 14:45 Poster C

Optical properties of neodymiumhydride from FIR to VUV — •Stefan Weber and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig

Many rare-earth metals show a metal to insulator transition when they are loaded with hydrogen. The dramatic changes in the optical and electronical properties are accompanied by a transition from an antiferromagnetic metal to a ferromagnetic semiconductor in the particular material system of neodymium.

Thin films of Nd have been grown onto different substrates by molecular beam epitaxy. They need a functional cap layer of Nb and Pd on top in order to allow hydrogen loading and to prevent the samples from corrosion in ambient air.

Temperature dependent transmission and reflection measurements have been performed with a FT-IR-spectrometer in the energy range of 5meV to 1eV. The structures in the spectra can unambiguously be assigned to hydrogen vibrations using the isotope effect which is a shift of the phonon frequencies by a factor of $\sqrt{2}$ by loading the samples with hydrogen or deuterium, respectively. The measurement of the optical properties of NdH_x is supplemented by UV/Vis-spectrometry which determines the optical band gap of the semiconductor. VUV ellipsometry in the energy range up to 10eV has been performed using synchrotron radiation at BESSY II which yields the pseudodielectric function. Simulating the thin film spectra with a multilayer model reveals the optical properties of NdH_x.

MM 20.39 Tue 14:45 Poster C

Electric field gradient and chemical bonding in intermetallic gallides — •Katrin Koch[1], Frank Haarmann[1], Klaus Koepernik[1,2], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]IFW, Dresden, Germany

The understanding of the metallic bond is still a challenging task. Here, we investigate experimentally and theoretically two series of compounds: the hexagonal MGa_2 with M=Ca,Sr,Ba and the tetragonal MGa_4 with M=Na,Sr,Ba. Ga forms a planar network of 3-fold coordinated atoms in MGa_2. In MGa_4 a 3-dimensional network of 4- and 5-fold coordinated Ga atoms is formed. The different bonding situations in these compounds indicate a flexibility of Ga with respect to the chemical bonding. We present a study of the electrical field gradient (EFG) for the different Ga sites in these materials. The quadrupolar coupling constants were measured by NMR, and the EFG was calculated using a DFT band structure code (WIEN2k). In comparison, the results of our calculation allow a unique assignment of the different signals to specific Ga sites. In addition, the calculations reveal that the EFG is very sensitive to internal structural parameters. For the optimized Ga positions (with respect to the total energy) we find excellent agreement of the measured and calculated EFG values. The large quadrupole coupling constants indicate clearly the covalent nature of the Ga bonds. Studying in detail the influence of the cations using the virtual crystal approximation we show that a simple point charge model can not be applied for this family of covalent metals.
The DFG SPP 1178 is acknowledged for financial support.

MM 20.40 Tue 14:45 Poster C

Paarkorrelationsspektroskopie an Festkörperoberflächen — •Robert Wallauer, Stefan Voss, Inka Lauter, Till Jahnke, Horst Schmidt-Böcking und Reinhard Dörner — Institut für Kernphysik, Frankfurt

Der Aufbau eines neuen Experimentes zum koinzidenten Nachweis zweier Elektronen emittiert durch ein Photon aus einer Festkörperoberfläche (Dopppelphotoemission DPE) soll hier präsentiert werden. Mit Hilfe dieser Technik gelang es der Gruppe Kirschner (Halle) mit grossen Erfolg die ersten Messungen an NaCl(100) und C60 durchzuführen und erstmals direkt die Elektron-Elektron Abstoßung sowie das Korrelationsloch sichtbar zu machen.

In unserer Gruppe wurde ein Paarkorrelationsspektrometer durch Mirko Hattass aufgebaut mit dem es erste erfolgreiche Messungen an Cu(100) gab. Ziel ist es nun die Technik auf Materialien mit stärkeren Korrelationseffekten, wie z.B. Supraleiter, zu übertragen und dabei hohe Impulsauflösung bei beiden Elektronen zu erreichen.

MM 20.41 Tue 14:45 Poster C

Optical investigations on $Fe_{1-x}Co_xSi$ single crystals using Raman spectroscopy under high pressure and far-infrared ellipsometry — •Ivan Jursic[1], Dirk Menzel[1], Pavlo Popovich[2], Alexander Boris[2], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelsohnstrasse 3, 38106 Braunschweig — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Single crystals of $Fe_{1-x}Co_xSi$ grown by the tri-arc Czochralski technique have been investigated using far-infrared spectroscopic ellipsometry. The band gap of the semiconductor FeSi, which is 33 meV at low temperatures, is filled with electrons when the temperature is increased. In the far-infrared range four infrared phonons can be identified. The full width of half maximum (FWHM) of these oscillators show different behaviour for the varying Co concentration. While for low Co content the FWHM of all phonons increases with rising temperature, for intermediate Co concentrations some of the peaks show a maxmimum in width as function of temperature. Also the oscillator strength has an unusual temperature dependence for certain phonons and concentrations. This striking behaviour is interpreted in terms of an electron–phonon interaction. The infrared data are compared to additional Raman investigations which have been performed with a diamond anvil pressure cell under high pressure.

MM 20.42 Tue 14:45 Poster C

Raman study of the semiconductor to metal phase transition in $Fe_{1-x}Co_xSi$ ($0 \leq x \leq 1$) — •Dirk Menzel[1], Ana Maria Racu[1], Thorsten Donig[1], Klaus Doll[2], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

A complete Raman spectroscopy study of $Fe_{1-x}Co_xSi$ with x between 0 and 1 is presented. All the 9 Raman active modes predicted by the factor group analysis are observed and assigned to the A, E and T symmetry species. A density functional calculation of the phonons in FeSi and in CoSi is consistent with the experimentally obtained frequencies of the Raman modes. When Co substitutes Fe in FeSi the most striking effect is a strong shift of the A-type mode of the transition element to a lower frequency. This shift is attributed to the different electronic surroundings of the vibrating atoms as follows: the interaction between the Co atoms is screened by the free electrons in the metallic compound CoSi in contrast to the semiconducting FeSi, leading to a decrease of the Raman mode frequency.

MM 20.43 Tue 14:45 Poster C

Post annealing effect on electrical transport properties and defect annealing of La 0.67 Ca 0.33 MnO 3 films grown on vicinal substrate — •Lan Yu[1,2], Hanns-Urich Habermeier[1], Pengxiang Zhang[1,2], and Jialin Shun[2] — [1]Max-Planck Institute for Solid State Research. Heisenberg str.1, 70569, Stuttgart,Germany — [2]Kunming University of Science and Technology,

La 0.67 Ca 0.33 MnO 3 thin films have been grown on 10°,15 *,20* vicinal cut LaAlO3 (100) substrates by PLD using identical growth conditions. The films have been subjected after characterization to a high temperature * high oxygen pressure annealing step. The films are characterized by transport measurements as well as dedicated X-ray analysis. As compared to as-grown films they showed drastic changes of the resistance- temperature curve , with enhancements of Tc from 257K to 291K and an obvious decreases of resistance. This effects are especially pronounced in films grown on 20 * miscut LAO. The as grown films show a systematic change of the resistivity and the peak temperature associated to the Curie temperature before annealing. The results are discussed with respect to the defect formation and other subsequent annealing arising from both, oxygen related as well as substrate-induced defects. Especially the role of the miscut angle and its relation to the defect formation will be highlighted and the role of oxygen reordering and strain relaxation upon annealing is discussed.

MM 20.44 Tue 14:45 Poster C

Wavefunction-based ab initio method for metals: applying the method of increments to magnesium — •Elena Voloshina and Beate Paulus — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Calculations based upon the incremental scheme [1], that is an expansion of the total correlation energy in terms of one-body, two-body, and higher contributions, have been performed on a variety of solids [2]. Metals require special treatment because of two distinct features. Since the conduction bands are only partially filled, we cannot construct well localized orbitals from them. Furthermore, we must deal

properly with charge screening which obviously is a correlation effect. One would expect that the metallic solid should be well described within DFT. Indeed, it is possible usually to select a DFT-functional that will yield good agreement of experimental and calculated properties. At the same time, it is well known, that the present DFT-based approaches are not amenable to systematic improvements. A starting point for the treatment of the many-body correlation effects in solids is a reliable HF SCF result for the infinite system. For magnesium HF model, ignoring the correlations, gives rather good agreement with experiment of one lattice parameter (c), but incorrect value for c/a ratio because of too high lattice parameter a. Application of the method of increments allow us not only to improve the HF values, but also explain the reason for these changes.

[1] H. Stoll, Phys. Rev. B 46, 6700 (1992).
[2] B. Paulus, Phys. Rep. 428, 1 (2006).

MM 20.45 Tue 14:45 Poster C

Electron correlation in 3*d* metals calculated with FLEX — •Andreas Gierlich[1], Arno Schindlmayr[1], Václav Drchal[2], and Stefan Blügel[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Prague 8, Czech Republic

The standard approach to material calculations, the density-functional theory (DFT) in its local-density or generalized gradient approximation, incorperates electronic correlations only rudimentarily. Our goal was to better understand the effects of electron correlation on the materials' properties of 3*d* transition metals which fall into the regime of intermediate correlation strength. The FLEX (fluctuation exchange) method, a diagrammatic technique that incorporates a range of two-particle scattering processes, allows a more accurate characterization of the correlation effects via the dynamic self-energy. We perform *ab initio* DFT calculations using the full-potential linearized augmented-plane-wave method and subsequently apply FLEX in a perturbative manner to explicitly include two-particle correlation for electrons in the *d* band. The self-energy is determined within the framework of dynamic mean-field theory. We present results for ferromagnetic (Fe, Co, Ni), antiferromagnetic (Cr) as well as non-magnetic 3*d* transition metals and compare the contributions of the different scattering channels for these groups of materials.

MM 20.46 Tue 14:45 Poster C

The Enatom in Simple Metals and Its pressure Evolution — •Jens Kunstmann[1], Lilia Boeri[1], and Warren Pickett[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Department of Physics, University of California Davis, Davis, California, 95616, USA

We present the first realization of the generalized pseudoatom concept introduced by Ball, and adopt the name enatom to minimize confusion. This enatom, which consists of a unique decomposition of the total charge density (or potential) of any solid into a sum of overlapping atomic-like contributions that move rigidly with the nuclei to first order, is calculated using (numerical) linear response methods, and is analyzed for both fcc Li and Al at pressures of 0, 35, and 50 GPa. These two simple fcc metals (Li is fcc and a good superconductor in the 20-40 GPa range) show different physical behaviors under pressure, which reflects the increasing covalency in Li and the lack of it in Al. The non-rigid (deformation) parts of the enatom charge and potential have opposite signs in Li and Al; it becomes larger under pressure only in Li. These preliminary results show that the enatom construction could be used to obtain a real-space understanding of the vibrational properties and electron-phonon interaction in solids.

MM 20.47 Tue 14:45 Poster C

The *GW* approximation in semi-infinite scattering setups — •Swantje Heers, Arno Schindlmayr, Daniel Wortmann, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

A proper description of electronic transport in nanoscale junctions must consider infinite systems without periodic boundary conditions. In addition, it is often desirable to include explicit electronic correlation, but the geometric setup makes the calculation of the electronic self-energy in the *GW* approximation much more complicated than for finite or periodic systems. We present an application of the *GW* approximation to a non-periodic model system with a simple one-dimensional scattering potential. The initial Green function is calculated with the embedding method in a finite region containing the scattering potential. The semi-infinite leads are taken into account by so-called embedding potentials. This Green function is the starting point for the *GW* approximation which requires solving Hedin's equations for the polarisation function, the dielectric function, the screened Coulomb interaction and the self-energy.

MM 20.48 Tue 14:45 Poster C

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 strongly on the composition.

MM 20.49 Tue 14:45 Poster C

^{119}Sn Mössbauer Spectroscopy of tin containing float glass — •Verena Jung[1], Ksenofontov Vadim[1], Claudia Felser[1], Maria Luisa Aigner[2], Thomas Pfeiffer[2], and Dirk Sprenger[2] — [1]Johannes Gutenberg - Universität, 55099 Mainz, Germany — [2]Schott AG, 55122 Mainz, Germany

According to the production process of float glasses tin is used as a common refining agent. Since the surface quality of the glass strongly depends on the local distribution of Sn-redox states, the influence of process parameters on Sn^{2+}/Sn^{4+} ratios and the assignment to their structural role in the glass network is extremely helpful. Therefore, glass compositions based on SiO_2-Al_2O_3-B_2O_3-CaO-SnO_2 were molten with additions of 0,1, 0,3 and 0,5 wt% SnO_2. All samples were tempered for 7 days at 1400^oC in N_2 and N_2-air mixtures with controlled p_{O2}-values of 10^{-2} and 10^{-5} bar, respectively. Hyperfine parameters for the tin nucleus in different structural units and their oxidation states were calculated from ^{119}Sn Mössbauer spectra, using theoretical simulations of electron densities and electric field gradients with the Wien2k software. Finally, the thermochemical impact of oxygen on the structure of Sn-bearing glasses is discussed.

MM 20.50 Tue 14:45 Poster C

A phase-field model to Investigate heterogeneous nucleation in peritectic materials — •Ricardo S. Siquieri[1] and Heike Emmerich[2] — [1]siquieri@ghi.rwth-aachen.de — [2]emmerich@ghi.rwth-aachen.de

Here we propose a phase-field approach to investigate the influence of convection on peritectic growth as well as the heterogeneous nucleation kinetics of peritectic systems. For this purpose we derive a phase-field model for peritectic growth taking into account fluid flow in the melt, which is convergent to the underlying sharp interface problem in the thin interface limit. Moreover, we employ our new phase-field model to study the heterogeneous nucleation kinetics of peritectic material systems. Our approach is based on a similar approach towards homogeneous nucleation in (Phys. Rev. Let. **88** 20 (2002)). We applied our model successfully to extend the nucleation rate predicted by classical nucleation theory for an additional morphological term relevant for peritectic growth. Further applications to understand the mechanisms and consequences of heterogeneous nucleation kinetics in more detail are discussed.

MM 20.51 Tue 14:45 Poster C

Calculation of transport coefficients from ab-initio methods — •Laurent Chaput[1,2], Pierre Pecheur[1], and Hubert Scherrer[1] — [1]Laboratoire de Physique des Matériaux, Nancy, France — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

A module to calculate transport properties of thermoelectric materials has been implemented. The system response is described within the framework of Boltzmann transport theory and the electronic structure of the system is taken as the one of Kohn-Sham electrons. This way we obtain the Onsager coefficients from which the thermoelectric tensor, the Hall tensor and the Lorenz coefficient are calculated. These quantities depend crucially on electron velocities. These are calculated using the spectral differentiation method. Therefore we obtain a very high accuracy while keeping the time-cost of the method relatively low. The other advantage of this method is that it is independent of

the basis used for the electronic structure calculation. The module can therefore be used with a variety of methods. In this contribution we consider the peculiar dependence with respect to temperature of the thermoelectric power of the MAX phase Ti_3SiC_2 . It has been reported to be essentially zero. The calculation of the thermoelectric tensor show that this come from a compensation between the components of the thermoelectric tensor. They are positive in the basal plane and negative along the z axis. We also derive a sum rule for the relaxation time. This simplify the calculation of the Hall tensor.

MM 20.52 Tue 14:45 Poster C

Tailoring phase change materials: Stoichiometrical trends in the Ge-Sb-Te system — •Michael Klein, Daniel Wamwangi, and Matthias Wuttig — I. Physikalisches Institut 1A, RWTH Aachen, 52056 Aachen, Germany

Phase change materials are widely used as the active layer in rewritable optical media. This layer can be reversibly switched with a laser beam between an amorphous and crystalline state. As there is a pronounced optical contrast between these two phases, this provides the possibility to write, read and erase data. The speed of this method is limited by the speed of crystallization, as crystallization is the slower process. One possibility to make this process faster is to change the composition of this active layer. Thus it is very interesting to investigate how the process of crystallization is affected by a variation of stoichiometry. Although phase change materials technology is already used, there is little knowledge of the phase change process itself. Today the usability of phase change materials is still identified by try and error methods. We will show stoichiometrical trends of different properties relevant for data storage, e.g. the crystallisation temperature, which governs the room temperature stability of the amorphous phase and thus is a measure for the data retention time.

MM 20.53 Tue 14:45 Poster C

Photoinduced ultrafast volume changes in intermediate valence solids — •momar diakhate and martin garcia — Theoretishe, physik,Universitat 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 gamma-Cerium and the subsequent ultrafast lattice expansion dynamics.

In particular we determine the thermodynamic and electronic properties of cerium 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.

By means of the Hugoniot theory the shock velocity variation in the surrounding (unheated) part of the sample was obtained and used to calculate the time dependence of the thermodynamic properties in the heated material.

MM 20.54 Tue 14:45 Poster C

Microstructure Characterization of Cu2MnAl Heusler-Type Alloys using SEM-EBSD and TEM — Tien Hung Luu[1,3], Huy Dan Nguyen[2], Vong Vo[2], •Steffen Schulze[3], and Michael Hietschold[3] — [1]Department of Physics, Vinh University, Nghean, Vietnam — [2]Institute of Materials Science, VAST, Hanoi, Vietnam — [3]Institute of Physics, TU Chemnitz, Chemnitz, Germany

Cu2MnAl heusler-type alloys prepared by the melt-spinning show soft magnetic behavior with a coercivity less than 1.6 kA/m and a Curie temperature as high as 600 K and after annealing a large negative magnetoresistance of more than 4%. In this work, we report microstructure investigations of these Cu2MnAl heusler alloys as-quenched and after annealing at 773 K for 24 hours using Electron Backscattered Diffraction (EBSD), Energy Dispersive X-ray Analysis (EDX), Selected Area Electron Diffraction (SAED) and High Resolution Transmission Electron Microscopy (HRTEM). The results show that the as-quenched sample is composed of Cu2MnAl in the fcc structure L21 only. These crystallites are of extremely elongated shape with sizes ranging between 1 to 3um in width and 5 to 15 um in length. After annealing we found two crystalline phases. The predominating one is still of L21 structure with grain sizes from 2 to 7 um but there is a Mn-rich phase too appearing in a wide variety of grain sizes. Some of them range between 10 and 20 nm and others are as big as 1 um in diameter. The appearance of these crystalline phases in the ribbons take essential effect on the magnetic and magnetoresistance properties.

MM 20.55 Tue 14:45 Poster C

Towards a combination of an electrical conductor with a thermal insulator — Ana Smontara[1], Igor Smiljanić[1], •Ante Bilušić[1,2], Benjamin Grushko[3], Sergiy Balanetskyy[3], Zvonko Jagličić[4], Stanislav Vrtnik[5], and Janez Dolinšek[5] — [1]Institute of Physics, Zagreb, Croatia — [2]Faculty of Science, Univ. of Split, Croatia — [3]Forschungszentrum Jülich, Germany — [4]Institute J. Stefan, Ljubljana, Slovenia — [5]Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

ϵ-phases in the Al-Pd-(Mn,Fe,Co,Rh, ...) alloys are complex intermetallics characterized by giant unit cells with quasicrystals-like cluster substructure. To see how the coexistence of two competing physical length scales affect their physical properties, we studied the magnetic, electrical, thermal transport and thermoelectric properties of the ϵ-Al-Pd-Fe, ϵ-Al-Pd-Co and ϵ-Al-Pd-Rh. Magnetic measurements reveal that the materials are diamagnetic, containing tiny fractions of magnetic transition-metal atoms (10-100 ppm). Electrical resistivity shows weak temperature dependence for $T = 4 - 300$ K. The thermal conductivity is low, comparable to that of thermal insulators amorphous SiO_2 and Zr/YO_2 ceramics at room temperature. While SiO_2 and Zr/YO_2 are also electrical insulators, ϵ-phases exhibit electrical conductivity typical of metallic alloys, so we deal with a combination of an electrical conductor with a thermal insulator. The thermoelectric power of the investigated ϵ-phase families is small, so that these materials do not appear promising candidates for the thermoelectric application. This work was done within the FP6 EU NoE "Complex Metallic Alloys".

MM 21: HV Nierlich

Time: Wednesday 14:00–14:30 Location: H16

Invited Talk MM 21.1 Wed 14:00 H16

XRD residual stress analysis: one of the few advanced physical measuring techniques that have established themselves for routine application in industry — •Wolfgang Nierlich and Jürgen Gegner — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

X-ray diffraction (XRD) provides a powerful testing tool for material response and failure analysis of Hertzian-loaded machine parts, like rolling bearings, camshafts or cogwheels, based on residual stress, martensite {211} line broadening, and retained austenite content. The conventional measuring procedure is improved by means of an iterative technique including a pre-analysis of the near-peak line-profile in order to substantially reduce the recording time. These achieved short measuring periods of 3 to 5 and around 10 min per residual stress value and retained austenite content, respectively, serve as precondition for routine industrial applications of XRD residual stress analysis over the last three decades within SKF. The adapted method is described in detail. The XRD line width represents a measure of material ageing within the lifetime cycle of a rolling bearing: calibration curves for the predominant (near-) surface and the classical sub-surface failure mode are available for material response analysis. A selection of concrete examples is given that describes different damage mechanisms.

MM 22: SYM Physics meets Industry

Time: Wednesday 14:45–19:55 Location: H16

MM 22.1 Wed 14:45 H16

Eine neue Bohr- und Auswertestrategie zur Bestimmung von Messunsicherheiten bei der Eigenspannungsermittlung nach dem inkrementellen Bohrlochverfahren — •Wulf Pfeiffer und Johannes Wenzel — Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg

Das Bohrlochverfahren ist als ökonomische Methode zur teilzerstörenden Eigenspannungsermittlung bekannt. Es beruht auf der Bestimmung von Dehnungsänderungen an der Oberfläche des Bauteils durch definierten Eingriff in das Eigenspannungsgleichgewicht (Bohren eines Sackloches). Ein wesentlicher Nachteil des Verfahrens ist, dass die Angabe der Messunsicherheit nur durch (meist nicht machbare) Wiederholungsmessungen möglich ist.

Es wurde ein Verfahren erarbeitet, das die Berechnung von Messunsicherheiten ohne Wiederholungsmessungen ermöglicht. Dazu wird für jeden Tiefenschritt das Bohrloch zusätzlich lateral aufgeweitet. Damit werden zusätzliche Dehnungsauslösungen zur Verfügung gestellt, die zur Berechnung einer Messwertstreuung herangezogen werden können. Der funktionale Zusammenhang zwischen den Dehnungsumlagerungen an der Bauteiloberfläche und inkrementeller Elimination spannungsbehafteter Volumenelemente wird durch Finite Elemente Modellierung bestimmt. Diese Kalibrierfunktionen können dann zur Berechnung diskreter Eigenspannungswerte für verschiedene Tiefen und Aufweitungen nach den bekannten linear-elastischen Ansätzen differenzieller Verfahren herangezogen werden. Durch Bohrversuche an einer Zugprobe unter bekannten Lastspannungen wurden die Ergebnisse der FE-Berechnungen verifiziert.

MM 22.2 Wed 15:05 H16

New Possibilities for X-ray Diffractometry — •Jörg Wiesmann, Christian Hoffmann, Jürgen Graf, and Carsten Michaelsen — Incoatec GmbH, Max-Planck-Str. 2, 21502 Geesthacht

During the last years the instrumentation for X-ray metrology has remarkably improved. There are numerous solutions for all components such as sources, optics and detectors. We present a new development for X-ray beams which we deliver in modules custom-built: the IμS - Incoatec Microfocus Source - is a high-brilliance X-ray source incorporating a 30W microfocus sealed tube together with a high-performance Montel Multilayer X-ray Optic. The IμS has the brilliance of a conventional 5.4-kW rotating anode system, but offers numerous benefits for example no moving parts, long lifetime without maintenance, air-cooling to name but a few. It can be integrated into various X-ray analytical systems using Cu or Mo radiation. The optics shape parallel as well as focused beams with different spot sizes. Data quality and ease of operation are strongly improved in applications such as biological and chemical crystallography and Small Angle X-ray Scattering (SAXS). For SAXS there is a factor of five intensity gain compared to a conventional sealed-tube setup. Finally we will give an outlook on further improvements of IμS. We invite users to discuss their requirements and share their ideas with us.

MM 22.3 Wed 15:25 H16

Advanced Residual Stress Investigation Utilizing Laboratory X-Ray Diffraction Instrumentation — •Lutz Brügemann and Jens Brechbühl — Bruker AXS, Karlsruhe, Germany

Different methods for the determination of material properties like hardness, tensile strength, and Young*s modulus are limited in their ability to characterize the performance of a material or a work piece entirely. However, X-ray diffraction based methods enable a non-destructive approach to the internal stress state of a work piece after even after heat treatment/hardening and/or grinding. Additionally, due to X-rays capability to penetrate the material, those diffraction based residual stress investigations allow determining volume information from some microns below the sample surface. By utilizing those methods even a depth profile/stress gradient can be studied.

Residual stress investigations are also of very high interest for wafer manufacturing. Thin Cu films or damascene Cu lines on Si-wafers need to be investigated with high lateral resolution (micro-diffraction). XRD2 using a 2-D photon counting detector is the right method allowing fast measurements although the signals are weak due to the small illuminated volume. Additionally, the commonly strong texture of the thin Cu lines can be recorded and considered simultaneously, and hence will not impede the stress measurements and data evaluation.

The goal of the presentation is to give a wider view of the principles of the residual stress investigations by using X-rays. By means of case studies the capabilities of laboratory instrumentation is presented.

MM 22.4 Wed 15:45 H16

The Deposition Process of Nanoscaled Multilayer Coatings for X-ray Optics — •Frank Hertlein, Jörg Wiesmann, Alexandra Oehr, Steffen Kroth, and Carsten Michaelsen — Incoatec GmbH, Max-Planck-Str. 2, 21502 Geesthacht

Incoatec develops, produces and sells X-ray optics with optimized properties. The optics consist of bent substrates with shape tolerances below 100nm, upon which multilayers are deposited with single layer thicknesses in the nanometer range and up to several hundreds of layer pairs. Additionally these multilayers were designed with lateral thickness gradients within +-1% deviation of the ideal shape. This means that a deposition precision in the picometer range is needed.

The talk will highlight how Incoatec designs, produces and characterizes these optics. We use sputtering methods for deposition, optical profilometry in order to characterize the shape and X-ray reflectometry to characterize the multilayers. The talk will emphasize the possibilities and limits of different in-situ and ex-situ metrology methods when manufacturing X-ray optics. Finally, ideas for new high precision metrology methods will be outlined.

15 min break

MM 22.5 Wed 16:20 H16

On the Application of SIMS for the Determination of Carbon Depth Profiles — •Peter-Joachim Wilbrandt[1], Jürgen Gegner[2], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, 97424 Schweinfurt, Germany

An industrially well-established method for the optimization of edge zone properties of steel components is carbon enrichment before hardening. Due to unreliable state-of-the-art process prediction, quality control and improvement of carburizing case hardening operations is essential. Additionally, detailed information on carbon distribution in edge zones is needed to assess decarburization during steel heat treatments and for computer simulations of carbon diffusion processes.

The standard methods for carbon concentration determination, like electron microprobe, glow discharge spectroscopy or hardness measurements, are limited regarding accuracy or spatial resolution. This motivated attempts to apply secondary ion mass spectroscopy (SIMS) as microchemical analysis technique for the determination of carbon profiles in ferrous materials.

The method is applied to metallographically prepared cross sections. After a detailed description of the measuring procedure, some representative applications to heat treatment technology, failure analysis and material science are discussed. A new method for the determination of carbon diffusivities in the austenitic phase of low-alloyed steels is presented.

MM 22.6 Wed 16:40 H16

High-temperature corrosion in waste incineration plants — •Barbara Waldmann, Bernhard Stöcker, Ferdinand Haider, and Siegfried Horn — Universität Augsburg

The corrosion of steels in heat exchangers of power plants is still not understood in all details. Especially in waste incineration plants the corrosion is a substantial technical and also economic problem. A corrosion probe was developed, which allowed to detect corrosion in real-time by performing potentiostatic analysis. The measurements were performed with three electrodes, two of which consisted of the steel (15Mo3) employed in the respective facility. Additionally the probe head was kept at the same temperature as the heat exchanger pipes to allow for a conclusion about the corrosion on the heat exchanger pipes in the facility. The measured corrosion rates agree well with those observed in the facility. In addition to these measurements, the influence of parameters like temperature, exhaust gas composition, or flow rate on the corrosion behaviour and the deposit composition were investigated by changing these parameters locally at the probe head.

MM 22.7 Wed 17:00 H16

Surface analysis of technological relevant samples — •Andreas Thissen — Voltastr. 5, 13355 Berlin, Germany

Electronic devices have revolutionized everyday life in industrial countries over the last decades. Recently two main tasks for research and development are dominant: miniaturization for sophisticated applications targetting at the nanoscale, and designing low cost large scale devices. In both fields the device performance is strongly determined by materials* quality, composition, combination and last but not least by processes at materials* interfaces. Nanostructures, minimization of material consumption and the need to improve device efficiencies consequently leads to the widespread focussing on thin film preparation. For thin film devices surface and interface analysis like photoelectron spectroscopy is an important tool for material and device characterization. Classical well defined model experiments already reveal important insights using highly integrated vacuum systems for analysis and preparation. But analysis of materials and devices under near environmental conditions and even in situ during operation is an inevitable future development to improve the significance of data for development and quality management. In this respect techniques like high pressure XPS, XPS from liquids and hard x-ray PES (HAXPS) are some of the challenging tasks for manufacturing companies for surface analytical equipment.

MM 22.8 Wed 17:20 H16

Fabrication and Mechanical Properties of Metal Thin Films — •Thomas Wübben[1], Gunther Richter[1], and Eduard Arzt[1,2] — [1]Max-Planck-Institut für Metallforschung, Heisenberg-Str. 3, 70569 Stuttgart — [2]Universität Stuttgart, Institut für Metallkunde, Heisenberg-Str. 3, 70569 Stuttgart

Nanoscale metallic materials and structures exhibit size-dependent mechanical properties, which deviate substantially from bulk values. Our research aims to understand and quantify this so-called size effect. Various experimental techniques have been established in our group over the last years. These include the classical substrate curvature technique as well as the newly developed in situ tensile tests with stress measurement by XRD methods. To retain control on quality and properties, all samples are produced in house by the thin film laboratory. This central scientific facility inside our institute offers different physical vapour deposition techniques, including magnetron sputtering and molecular beam epitaxy. An extensive data base of the mechanical properties of the technologically important metals Cu, Al and Ag could be built up this way. The presentation will give an overview about the production and testing possibilities in our group. It will finally highlight the major technical challenges for future research and what we request from industry.

MM 22.9 Wed 17:40 H16

Flap Simulation and Testing System for the A400M Airbus — •Klaus Metzger[1] and Peter Scholz[2] — [1]imc Meßsysteme GmbH, Voltastr. 5, 13355 Berlin — [2]ADDITIVE GmbH, Max-Planck-Str. 22b, 61381 Friedrichsdorf

The measurement system consists of an actual Airbus A400M wing, combined with a virtual simulated wing. It is designed to measure the electrical and mechanical systems of the entire wing flap system. In addition to the hundreds of analog signals (including force, temperature, and voltage), it is important to record additional information, including the safety critical data on the ARNIC bus and other modern industrial serial data buses.

In summary, the whole system can handle and store a data volume of several mega words per second, from the various different data sources. The control and response of the missing wing is simulated such that the airplane systems behave as if it works with a complete system. This makes it possible to simulate and analyze all flight relevant situations. For data storage, PC systems with terra-byte capacities are used. A user friendly configuration and analysis interface, allowing operations simultaneously on six systems completes the system.

15 min break

MM 22.10 Wed 18:15 H16

Quantitative elastic modulus measurement at the nanoscale using atomic force microscope — •Udo Volz[3], Sergey Belikov[1], Sergei Magonov[1], Natalia Erina[1], Lin Huang[1], Craig Prater[1], Valeriy Ginzburg[2], Gregory Meyers[2], Robert McIntyre[2], and Hamed Lakrout[2] — [1]Veeco Instruments Inc., 112 Robin Hill Road, Santa Barbara, CA 93117, USA — [2]Dow Chemical Company, Analytical Sciences 1897E Building, Midland, MI 48667, USA — [3]Veeco Instruments GmbH, Dynamostrasse 19, D-68165 Mannheim, Germany

Quantitative studies of the elastic modulus of homogeneous polymer materials in a wide modulus range and recognition of the individual components and the interphases in heterogeneous systems with the AFM-based cantilever nanoindentation method will be presented.

MM 22.11 Wed 18:35 H16

Some new application aspects of scanning electron microscopy — •Hans-Georg Braun and Evelyn Meyer — Leibnitz Institute of Polymer Research Dresden, Max Bergmann Center of Biomaterials, D-01069 Dresden, Hohe Strasse 6

Scanning electron microscopy is a well established tool for the material scientist. Recent developments in SEM instrumentation allow the SEM operation at low (E<1 KeV) electron energies which overs remarkable possibilities in imaging ultrathin (t<10 nm) layers, especially polymer layers with high image contrast. In addition low operation voltage allows imaging of non-conducting materials such as polymer, ceramics or glass without electrical charging. The integration of tiny manipulation tools into the SEM makes the SEM a nano- or microlaboratory. The manipulation tools inside the SEM allow an interaction with the sample under direct observation at high magnifications. Tiny things can be moved, particles be separated and tools for measuring purpose can be adjusted under visual control.

MM 22.12 Wed 18:55 H16

Modulation of stress-GBD curves of a polycristalline fibre mat using a micromechanic model — •Florian Wolferseder[1], Ferdinand Haider[2], and Uwe Tröger[3] — [1]Universität Augsburg, Institut für Physik — [2]Universität Augsburg, Institut für Physik, Experimentalphysik I — [3]Firma ArvinMeritor, Augsburg, Deutschland

Polycrystalline fibre mats are used to support ceramic substrates in catalytic converters and diesel particulate filters. Under compressive loading the fibre mats show a non-linear stress-strain behaviour. The stress-GBD (gap bulk density) curves follow a power-law relationship in accordance with several models. The models predict an exponent of the power law higher 3, depending on the architecture of the fibre network. In-situ-deformation in a SEM on the fibre mat were conducted in order to verify the assumptions of the model and the results of the compression tests. Another aim has been to find an empirical formula of the stress-time behaviour for long time relaxation experiments.

MM 22.13 Wed 19:15 H16

On the Feasibility of Nitrogen Concentration Measurements in Steels by SIMS — Nicolas Bontems[1], •Peter-Joachim Wilbrandt[1], Jürgen Gegner[2], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, 97424 Schweinfurt, Germany

Besides the carbon distribution, which permits adjusting constant or varying hardness and microstructure across the wall thickness, nitrogen enrichment represents an effective method to improve the edge zone properties of steel components. More stable martensite is formed and higher retained austenite contents can be achieved. Since recent developments turned SIMS into a powerful technique for industrial routine carbon profile determination, the attempt was made to trace nitrogen parallel to carbon concentrations. Such a combined microanalytical measuring tool is most useful for quality control and process improvement of upcoming carbonitriding heat treatment technologies.

Five specimens with different carbon and nitrogen contents were analyzed. First tests yield good reproducibility of the counting rates and, thus, the general usability of the method. A systematic analysis of the mass spectra shows that nitrogen atoms can best be detected as negatively ionized molecule CN. As the amount of detected CN molecules is proportional to the carbon content, it was concluded that the CN/C ratio is representative of the nitrogen concentration. Comparison of such ratios with nitrogen content data proved this to be valid.

MM 22.14 Wed 19:35 H16

Measurement of Nano ordered structure in Biological macromolecules using SAXS technique — •Dillip Kumar Bisoyi — Department of physics, National Institute of Technology Rourkela, Rourkela-769008(INDIA)

Biological macromolecules play an important role in the living world. So to know the macromolecules and to characterize them from nano

ordered structure available in them is an important problem before the scientific community. There are various techniques available to solve such problems. One such informative tool is the Small Angle X-ray Scattering (SAXS), where nano ordered structure can be well resolved and hence informative solutions can be extracted and utilized to solve various problems related to biological macromolecules. Out of many biological macromolecules of importance to study, I have emphasized here human bone, because it has very complex structure, which was studied at nono order and discussed to some depth in this article. The nano ordered structure evaluated are in good agreement with the findings referred else where.

MM 23: Nano structured materials I

Time: Wednesday 14:45–16:15 Location: H4

MM 23.1 Wed 14:45 H4

New method for single wall carbon nanotube growth — •Petr Nozar[1], Roberto Danieli[2], Viliam Vretenar[1], Riccardo Lotti[2], and Carlo Taliani[1,2] — [1]Istituto per lo Studio dei Materiali Nanostrutturati, CNR, Via P. Gobetti, 101, 40129 Bologna, Italy — [2]Organic Spintronics, Srl, Via P. Gobetti, 101, 40129 Bologna, Italy

In the present contribution we report on a novel preparation method for Single Wall Carbon Nanotubes (SWCNT). The procedure is based on brand-new system of Pulsed Plasma Deposition (PPD) developed by Organic Spintronics, Srl. PPD for SWCNT growth represent a synthesis of methods based on a production of catalyst nanoparticles (nickel-cobalt) by plasma heating and CVD ones. The SWCNTs obtained by reported procedure are isolated (not in bundles) with very narrow distribution of diameters and almost free of amorphous carbon and graphite impurities.

MM 23.2 Wed 15:00 H4

Nanowire Devices formed by Wet Chemistry — •Mady Elbahri, Khaled Hirmas, and Rainer Adelung — Chair for Multicomponent Materials, Technical Faculty, University of Kiel, Germany

The electronic structure of polycrystalline nanowires is modified if molecules attach on their surfaces. Employing this effect, sensor demonstration devices have been built. For example, interparticle boundaries of metallic nanowires have been used to sense different gases [1]. Semiconductor nanowires can be utilized as gates in field effect transistors to detect electric fields caused by atoms around them [2]. Even though these demonstrators show the potential of nanowires in sensing technology, simple and cost effective methods suitable for mass fabrication are still not established. Surprisingly, we found that nanowires formed by wet chemical methods [3] can be reproducibly aligned with high precision. Therefore, the nanowire fabrication is not performed in a beaker, but directly on a silicon chip surface. By using masks with relatively large structure sizes (>0,05 mm), we show how wet chemically produced metal (Ag) as well as semiconducting (ZnO) nanowire patterns like rings and arrays of parallel wires form at well defined positions on a silicon chip surface. Beside the details of the fabrication scheme, the electrical and electronic properties of the devices will be discussed.

[1] B. J. Murray, E. C. Walter, and R. M. Penner, Nano Lett. 4, 665, (2004). [2] F. Patolsky and C. M. Lieber, Mat. Today 8(4), 20 (2005). [3] M. Elbahri, R. Adelung, and D. Paretkar, Deutsches Patentamt, DE 10 2005 060 407.2 (2006).

MM 23.3 Wed 15:15 H4

Low temperature synthesis of Zn nanowires by physical vapor deposition — •Philipp Schroeder, Michael Kast, and Hubert Brückl — Austrian Research Centers GmbH ARC, Nano-Systemtechnologies, Donau-City-Straße 1, A-1220 Wien, Austria

We demonstrate catalytic growth of zinc nanowires by physical vapor deposition at modest temperatures of 125-175°C on various substrates. In contrast to conventional approaches using tube furnaces our home-built growth system allows to control the vapor sources and the substrate temperature separately. The silicon substrates were sputter coated with a thin gold layer as metal catalyst. The samples were heated to the growth temperature and subsequently exposed to the zinc vapor at high vacuum conditions. The work pressure was adjusted by the partial pressure of oxygen or argon flow gas. Scanning electron microscopy and atomic force microscopy characterizations revealed that the nanowires exhibit straight, uniform morphology and have diameters in the range of 50-350 nm and lengths up to 70 μm. The Zn nanowires grow independently of the substrates crystal orientation via a catalytic vapor-solid growth mechanism. Since no nanowire formation was observed without gold coating, we expect that the one-dimensional growth is initiated by a surface reactive Au seed. ZnO nanowires can be produced in the same preparation chamber by oxidation at 500°C in 1atm (80% Ar, 20% O2) for 1 hour. ZnO is highly attractive for sensor applications.

MM 23.4 Wed 15:30 H4

Electrical Properties and Oxidation Behavior of Nanowires — •Seid Jebril, Kittitat Subannajui, Mady Elbahri, and Rainer Adelung — Chair for Multicomponent Materials, Technical Faculty, University of Kiel, Germany

The integration of nanowires into silicon chips, microstructured by conventional lithography, is still a difficult task. Either the procedures are costly or they suffer from small throughput. Lately, we suggested a cost effective method based on thin film fracture [1]. We demonstrate that this can be adopted to form reproducible nanowires between micro-contacts formed by standard lithography. Therefore, simple geometrical objects like microstructured photo-resist bars were integrated in a layout of a silicon chip. Exposing the bars to stress leads highly reproducible fracture patterns that are used as templates for a successive nanowire fabrication step. We show microchips containing integrated Au and Ni nanowires. The conductivity behavior as a function of the wire diameter and temperature is discussed, and the changes in current due to field induced as well as normal oxidation of Ni nanowires is investigated.

[1] M. Elbahri, S. K. Rudra, S. Wille, S. Jebril, M. Scharnberg, D. Paretkar, R. Kunz, H. Rui, A. Biswas, R. Adelung, Adv. Mater. 18, 1059 (2006).

MM 23.5 Wed 15:45 H4

Winkelabhängigkeit der Koerzitivfeldstärke bei Nickel-Nanostäben — •Annegret Günther, Stefan Monz, Andreas Michels, Andreas Tschöpe, and Rainer Birringer — FR 7.3 Technische Physik, Universität des Saarlandes, Geb. D 2.2, D-66123 Saarbrücken

Nickel-Nanostäbe wurden mittels des Elektrodepositionsverfahrens in eine poröse Aluminiumoxidschicht abgeschieden. Durch geeignete Wahl der Prozessparameter (Anodisierungsspannung, Stromdichte, Zeit) konnten Stäbe mit einem mittleren Durchmesser D zwischen etwa $15-100$ nm, einer Länge L zwischen $50-500$ nm und variablem ("center-to-center") Abstand hergestellt werden. Die Stabensembles wurden mittels Elektronenmikroskopie und VSM-Magnetometrie charakterisiert. Bei den magnetischen Messungen lag der Schwerpunkt auf der Untersuchung der Abhängigkeit der Koerzitivfeldstärke H_C vom Winkel Θ zwischen angelegtem Magnetfeld und Stabachse sowie von den Abmessungen (D und L) der Nanostäbe. Insbesondere galt unser Interesse dabei dem Studium des Übergangs vom "coherent rotation" zum "curling" Magnetisierungsumkehrprozess, der für Ni bei einem kritischen Stabdurchmesser von ungefähr 20 nm erwartet wird.

MM 23.6 Wed 16:00 H4

Field emission properties of bare and gold coated metallic nanowires grown in polymer ion-track membranes — •Arti Dangwal[1], Günter Müller[1], Florian Maurer[2], Joachim Brötz[2], Hartmut Fuess[2], and Christina Trautmann[3] — [1]FB C Physics Department, University of Wuppertal, D-42097 Wuppertal, Germany — [2]epartment of Material and Earth Sciences, Darmstadt University of Technology, D-64287 Darmstadt, Germany — [3]Gesellschaft für Schwerionenforschung (GSI), D-64291 Darmstadt, Germany

We have measured the field emission (FE) properties of randomly distributed free-standing bare and gold coated Cu and Ni nanowires grown electrochemically into the pores of etched ion-tracked polycarbonate membranes [1]. The emission site density and current distribution of nanowires were measured with the field emission scanning micro-

scope. Onset fields of some V/μm for nA current were observed for all samples. In the best case, at 5 V/μm bundled Cu and Au-coated Ni nanowires yielded more than 10^5 emitters/cm2. Average field enhancement factors for all measured samples lie in the range 245-331, which correspond well to the field enhancement estimated from their cylindrical shape in SEM images [2]. Au-coated bundled Cu nanowires sample showed best results among all measured samples in terms of carrying high and stable FE currents, i.e. most of the emitting sites produced FE currents in 10 -35 μA range without destruction.

[1] F. Maurer et al., Nuclear Instruments Methods in Physics Research B 245, 337 (2006).

[2] A. Dangwal et al., subm. to JVST B.

MM 24: Nano structured materials II

Time: Wednesday 16:45–18:15 Location: H4

MM 24.1 Wed 16:45 H4

Atomistic simulation of carbon nanostructures in electronic nonequilibrium — •Harald O. Jeschke[1], Aldo H. Romero[2], Traian Dumitrica[3], and Martin E. Garcia[4] — [1]Institut für Theoretische Physik, Universität Frankfurt, Germany — [2]CINVESTAV Querétaro, Querétaro, México — [3]Department of Mechanical Engineering, University of Minnesota, USA — [4]Theoretische Physik, Universität Kassel, Germany

We analyze the response of carbon nanostructures to laser induced nonequilibrium by performing molecular dynamics simulation on time dependent potential energy surfaces. We observe that typical defects in carbon nanotubes become instable upon excitation of electron hole pairs, and the nanotubes heal. We also find that the excitation of coherent phonons can be exploited in capped carbon nanotubes to achieve a clean separation of the nanotube cap and body. In a broad investigation of the stability of single wall nanotubes upon laser irradiation we find interesting dependencies on nanotube diameter and on the laser pulse parameters.

MM 24.2 Wed 17:00 H4

Radial distribution function as a tool to analyse nanotubes chiralities — •Pedro Ojeda[1], Mauricio Terrones[2], Humberto Terrones[2], Darin Hoffman[3], Thomas Proffen[3], Anthony Cheetham[4], and Martin Garcia[1] — [1]Theoretische Physik FB 18, Universitaet Kassel — [2]Advenced Materials Department, IPICyT, SLP, Mexico — [3]Manuel Lujan Jr. Neutron Scattering Center, Los Alamos, NM 87545, USA — [4]Materials Research Laboratory, University of California, Santa Barbara, CA 93106-5121, USA

The radial distribution function (RDF) of different single walled carbon nanotubes (SWCNTs) has been calculated showing characteristic patterns. Features related to diameter, chirality and doping in these nanostructures are analyzed. We also investigate the induced chirality of two samples, prepared with the chemical vapor deposition (CVD) method and the high pressure Co conversion (HIPCo) procedure, respectively, by comparing the experimental RDF signal obtained from the neutron scattering technique with the RDFs of our simulations. We found armchair and zigzag nanotubes in the sample, but we cannot discard the presence of other chiralities. We believe that this is a useful method to study chiralities induced by different methods of production. Data up to $Q = 30$ Å^{-1} were used in the Fourier transform, giving a high real space resolution of $\Delta r \sim 0.2$ Å.

MM 24.3 Wed 17:15 H4

A general approach to control the radius and the chirality of nanotubes — •Jens Kunstmann[1], Alexander Quandt[2], and Ihsan Boustani[3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Institut für Physik der Ernst-Moritz-Arndt-Universität Greifswald, Domstraße 10a, 17489 Greifswald — [3]Bergische Universität Wuppertal, FB C Mathematik und Naturwissenschaften, Gaußstraße 20, 42097 Wuppertal

The success of future nanotechnologies will strongly depend on our ability to control the structure of materials on the atomic scale. For nanotubes it turns out that one of their structural parameters - the chirality - may not be controlled during synthesis. We explain the basic reason for this defect and show that novel classes of nanotubes like boron nanotubes, related to sheets with anisotropic in-plane mechanical properties, may overcome these problems. Our results further suggest that extended searches for nanomaterials similar to pure boron will allow for one of the simplest and most direct ways to achieve structure control within nanotechnology.

MM 24.4 Wed 17:30 H4

Molecular dynamics simulation of the formation of iron-platinum clusters — •Norbert Lümmen[1] and Thomas Kraska[2] — [1]Institute for Physics and Technology, University in Bergen, Norway — [2]Institute for Physical Chemistry, University Cologne, Germany

The formation of iron-platinum clusters from the vapour phase is investigated by molecular dynamics simulation. The metal interaction is modelled by an embedded atom potential method. Argon is added as carrier gas for removing the condensation heat from the system.

The first step of the particle formation is homogeneous nucleation. We found that in the iron-platinum system pure platinum nucleation takes place to a certain extent. We attribute this effect to the difference in cohesive energies of the two substances leading to heat transfer from platinum clusters to iron atoms which makes it less likely for them to condense at the same time due to their high temperature. This observation is in agreement with experimental results on the palladium-platinum system in the literature.

The proceeding growth process comprises surface growth, coalescence and agglomeration. The analysis of the atomic order shows that the disordered tetragonal face centred structure dominates. In order to obtain the ordered $L1_0$ structure we have run sinter simulations with different temperature programs applied to the carrier gas argon. Furthermore different cluster sizes ranging from 3 nm to 3.5 nm are analysed with respect to the structure formation. At the current state the onset of $L1_0$ formation can be observed.

MM 24.5 Wed 17:45 H4

Platinum deposition on polyethylene films investigated by molecular dynamics — •Thomas Kraska and Roberto Rozas — Institute for Physical Chemistry, University Cologne, Luxemburger Str. 116, 50939 Köln, Germany

The growth mechanisms of platinum clusters on and in a polyethylene film is investigated by molecular dynamics simulation. This system has been chosen as a model system with a relatively simple polymer. Platinum is modelled by the embedded atom method and polyethylene by a united atom model with flexible bonds, angle potential, and torsion potential for the intramolecular two-, three-, and four-body interactions. The intermolecular interaction is modelled by a Lennard Jones potential. Furthermore argon is added as carrier gas which removes heat from the vapour phase by collision with the platinum atoms and the polymer surface. An equilibrated polyethylene film is set in the middle of a rectangular box. The gas phase volume of the box is filled with platinum and argon atoms. Once the simulation is started clusters form in the vapour phase as well as on and in the polyethylene film.

Simulations at different platinum vapour phase densities are analysed with respect to the growth mechanism. General agreement is found with metal/polymer systems investigated experimentally in the literature. At higher platinum supersaturation less platinum diffuses into the polymer film. This is due to homogeneous nucleation the vapour phase leading to large clusters, which less likely diffuse into the polymer.

MM 24.6 Wed 18:00 H4

Balancing the White Light Shade of Dual-Color Emitting Nanocrystals — •Sergiy Mayilo[1], Sameer Sapra[2], Thomas Klar[1], Andrey Rogach[1], and Jochen Feldmann[1] — [1]Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians Universität München, Germany — [2]Physical Chemistry Group, Technische Universität Dresden, Germany

Semiconductor nanocrystals (NCs) are highly fluorescent with fluorescence quantum efficiencies as high as 80%, being ideal candidates for use in white light emitting devices. Simple mixing of red, green and blue emitting NCs may lead to undesirable changes in color during the lifetime of the device due to different temporal stabilities of the

components. Here we present the generation of white light from core-shell-shell CdSe/ZnS/CdSe NCs [1]. These particles have two emission lines: blue (500 nm) from the CdSe shell and orange (612 nm) from the CdSe core. The ZnS layer is used as a spacer between the two emitting regions. The shade of the white light can be controlled during synthesis by varying the thickness of the CdSe shell. The relative intensities of both emission lines are also determined by intra-nanocrystal energy transfer. When the colors are well matched the resulting emission appears as pure white light. The synthesized NCs have 30% quantum efficiency.

[1] S. Sapra, S. Mayilo, T.A. Klar, A.L. Rogach, J. Feldmann, Bright white light emission from semiconductor nanocrystals: by chance and by design, Advanced Materials (in press)

MM 25: Electronic properties II

Time: Wednesday 14:45–16:15 Location: H6

MM 25.1 Wed 14:45 H6

Valence-dependent Analytic Bond-order Potential for Transition Metals — •Ralf Drautz and David Pettifor — Department of Materials, Unversity of Oxford, Oxford, UK

An analytic interatomic bond-order potential (BOP) is presented that depends explicitly on the valence of the transition metal element [1]. This analytic potential predicts not only the structural trend from hcp to bcc to hcp to fcc that is observed across the non-magnetic 4d and 5d transition metal series, but also the different ferromagnetic moments of the alpha (bcc), gamma (fcc) and epsilon (hcp) phase of the 3d transition metal iron as well as the difference between the ferromagnetic and anti-ferromagnetic states. In addition, this new potential includes a correct description of alloy bonding within its remit. In this talk we discuss how the potential is derived from the tight-binding electronic structure and demonstrate that it may be regarded as a systematic extension of the second-moment Finnis-Sinclair potential to include higher moments.

[1] R. Drautz and D.G. Pettifor, Phys. Rev. B 74, 174117 (2006).

MM 25.2 Wed 15:00 H6

Effects of local interactions on transport through interfaces — •Frank Freimuth, Daniel Wortmann, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

The embedding technique provides a tool to calculate the Green function of the interface region of planar junctions suitable for application within DFT ab-initio studies of electronic transport. Our implementation of the embedding technique is based on the full-potential linearized augmented plane wave (FLAPW) method which does not make any approximations to the potential. In this talk, we give an outline of how the local Coulomb interaction may be taken into account within the embedding Green function approach through the local contribution to the self-energy. Wannier functions constructed from the DFT Bloch states of the interface provide a localized set of basis functions adequate for the calculation of many-body effects using many-body techniques formulated for lattice systems.

MM 25.3 Wed 15:15 H6

Conserving GW calculations for small metal clusters — •George Pal, Yaroslav Pavlyukh, Hans Christian Schneider, and Wolfgang Hübner — Fachbereich Physik, Technische Universität Kaiserslautern, P.O. Box 3049, 67663 Kaiserslautern, Germany

We present a GW-like approach for the quasiparticle energies and lifetimes of the closed-shell Na_4, Na_9^+ and Na_{21}^+ clusters. The screened Coulomb potential is constructed directly from the density-density correlation function, which is the functional derivative of a conserving single-particle Green's function with respect to an external potential. The density-density correlation function is obtained numerically by solving a quantum kinetic equation for the linear response of the system subject to a weak external perturbation. The conserving nature of our approach is shown by explicitly evaluating the f-sum rule. Analyzing the quasiparticle spectral functions, we find pronounced differences in the peak positions and broadenings when comparing our results with the self-consistent GW-RPA approach, which is not conserving at the two-particle level.

MM 25.4 Wed 15:30 H6

Is black phosphorous really a semiconductor? — •Alim Ormeci and Helge Rosner — Max-Planck-Institut CPfS, Dresden

Black phosphorous in the A17 orthorhombic structure (space group 64) is known to be a narrow-band-gap semiconductor (E_g = 0.3 eV) at ambient pressure. However, our recent electronic structure calculations based on various state-of-the-art first-principles, all-electron, full-potential codes have revealed that there is actually no gap in the electronic band structure of black phosphorous! Both LDA and GGA calculations give one small electron, and one small hole pocket around the **k**-point corresponding to $2\pi/b$ along the longest orthorhombic axis b. Thus, according to these very accurate calculations black phosphorous should be a compensated (semi)metal with very small $N(E_F)$ values in a wide range of unit cell volumes, at least between $0.90\,V_0$ and $1.15\,V_0$, where V_0 is the ambient pressure volume. The finding that the computed Fermi surface areas are very small has both computational and experimental implications. On the computational side, very fine sampling of the Brillouin zone is necessary in order to have a correct and converged result. On the experimental side, the implied low carrier concentration may introduce complications. We suggest new experiments such as photoemission, conductivity and de Haas-van Alphen measurements, to be performed on very pure, well-characterized single crystals of black phosphorous for testing the prediction regarding the existence of these small Fermi surfaces.

DFG Emmy Noether Programm is acknowledged for support.

MM 25.5 Wed 15:45 H6

The lattice structure of Zn, Cd, and Hg — Nicola Gaston and •Beate Paulus — MPI fuer Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany

Mercury condenses at 233 K into the rhombohedral structure with a bond length a=3.005 Ang and an angle of 70.53 degree. In contrast, zinc and cadmium adopt the hexagonal close-packed (hcp) structure, but with an anomolous c/a ratio which is far from ideal hcp. Density functional methods fail to describe either of these structures accurately. An application of the method of increments [1] to these metals, including correlation via coupled cluster calculations on finite fragments of the solid, allows the systematic inclusion and comparison of the competing effects that leads to the observed structures [2].

[1] B. Paulus, Phys. Rep. 428, 1 (2006). [2] N. Gaston, B. Paulus, K. Rosciszewski, P. Schwerdtfeger and H. Stoll, Phys. Rev. B 74, 094102 (2006)

MM 25.6 Wed 16:00 H6

Boron/Carbon ordering in layered MB_2C_2 compounds — Sergii Khmelevskyi, Peter Mohn, and •Josef Redinger — Inst. f. Allgemeine Physik, Vienna University of Technology, Getreidemarkt 9/134, A-1060 Vienna, Austria

Superconductivity in layered diboride dicarbide materials has been observed in YB_2C_2 and LuB_2C_2, but not in LaB_2C_2. Starting from our previous ab-initio DFT work on YB_2C_2 [1], where we showed that metallic conductivity in the stable $P4/mbm$ structure is due to Y d-bands partially hybridized with p_z-states from the boron-carbon planes, we present new results on the electronic structure of various layered boro-carbides such as CaB_2C_2, ScB_2C_2, SrB_2C_2, YB_2C_2, LaB_2C_2 and LuB_2C_2. We concentrate on the ordering of B and C in the layers and the impact of $d-p$ hybridization which seems to decide the actually observed structures. Except ScB_2C_2 which favours a 5-7 ring boron-carbon network ($Pbma$) all the others prefer 4-8 ring networks with alternating B and C atoms within the boron-carbon layer and a B-B (C-C) - like ($P4/mbm$) or B-C (C-B) - like ($I4/mcm$) layer stacking along the c-axis. Apparently, $d-p$ hybridization (YB_2C_2, LaB_2C_2 and LuB_2C_2) tips the scale in favour of $P4/mbm$, whereas CaB_2C_2 and SrB_2C_2 remain $I4/mcm$.

[1] S. Khmelevskyi, P. Mohn, J. Redinger, and H. Michor, Supercond. Sci. Technol. 18, 422-426, (2005).

MM 26: Electronic properties III

Time: Wednesday 16:45–18:15 Location: H6

MM 26.1 Wed 16:45 H6

Density matrix functional theory versus density functional theory: application to the Hubbard model — •Ryan Requist and Oleg Pankratov — Lst. für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg

While the Hohenberg-Kohn theorem was long ago extended to prove a one-to-one correspondence between the first order reduced density matrix (RDM) and a nonlocal external potential [1], only recently have approximate RDM functionals been applied to systems such as atoms, small molecules, and the homogeneous electron gas. We study a two site Hubbard model which is exactly solvable; therefore, it provides a context for an explicit comparison of the density functional (DFT) and RDM functional approaches. In the RDM formalism, the Kohn-Sham (KS) system generally has fractionally occupied states, and all of these are degenerate, which is quite different from the common KS-DFT approach. The iteration of the self-consistent RDM equations leads to a nonlinear discrete map. Due to the degeneracy of the KS spectrum of the ground state RDM, an analogue of the Jahn-Teller theorem implies that the ground state is an unstable fixed point of the iteration map. The RDM energy functional constructed here may be useful for studying strongly correlated systems.
[1] T. L. Gilbert, Phys. Rev. B **12**, 2111 (1975).

MM 26.2 Wed 17:00 H6

topolgical defects in the crystalline state of the non-uniform density one component plasma — •adil mughal and mike moore — department of physics and astronomy, university of manchester, manchester, m13 9pl, u.k.

We study the ground state properties of classical Coulomb charges moving on a plane but confined either by a circular hard wall boundary or by a harmonic potential. The charge density in the continuum limit is determined analytically and is non-uniform. Because of the non-uniform density there are both disclinations and dislocations present and their distribution across the system is calculated and shown to be in agreement with numerical studies of systems of N charges, where values of N up to 5000 have been studied. A consequence of these defects is that although the charges locally form into a triangular lattice structure, the lattice lines acquire a marked curvature. A study is made of conformal crystals to illuminate the origin of this curvature. The scaling of various terms which contribute to the overall energy of the system of charges viz, the continuum electrostatic energy, correlation energy, surface energy (and so on) as a function of the number of particles N is determined. "Magic number" clusters are those at special values of N whose energies take them below the energy estimated from the scaling forms and are identified with charge arrangements of high symmetry.

MM 26.3 Wed 17:15 H6

Ionicity of $Fe_{1-x}Co_xSi$ single crystals from far-infrared spectroscopic ellipsometry — •Dirk Menzel[1], Pavlo Popovich[2], Alexander Boris[2], Matthias Neef[3], Klaus Doll[2,3], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

The nonmagnetic narrow-gap semiconductor FeSi transforms into a ferromagnetic metal by doping between 5 at.% and 80 at.% Co. High-quality tri-arc Czochralski grown $Fe_{1-x}Co_xSi$ single crystals were investigated by spectroscopic ellipsometry in the far-infrared spectral range between 100 and 700 cm^{-1}. Four infrared active T-modes are observed at 206, 330, 351, and 459 cm^{-1} for FeSi. The best fit of the dielectric function is achieved with a sum of Fano oscillators reflecting a coupling of the optical phonons with electronic excitations. Interestingly, at Co concentrations $x > 0.05$ the phonons remain visible although they should be screened by free carriers as expected in a metal. This is even more surprising since the Szigeti effective charge is lower than $0.1e$ for all the investigated Co concentrations whereas the Born effective charge is $3.0e$. For pure FeSi the indirect optical band gap is 33 meV which decreases with increasing x and closes at 5 at.% Co.

MM 26.4 Wed 17:30 H6

Optic phonon anomaly as a precursor to polaron formation in a layered CMR manganite — •Dmitry Reznik[1], Frank Weber[1,2], Nadir Aliouane[3], Dimitri Argyriou[3], Marcus Braden[4], and Winfried Reichardt[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany — [3]Hahn-Meitner Institut, Glienicker Straße 100, D-14109 Berlin, Germany — [4]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln, Germany

We found evidence of a precursor effect to polaron formation in the bond stretching phonons in the bilayer CMR manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ at 10K. Neutron scattering measurements of these phonons in the XX0 direction show that both the transverse and longitudinal branches broaden abruptly from X=0.15, where they are resolution limited, to X=0.25 where FWHM=13meV. They then narrow again on approach to the zone boundary (X=0.5). The shell model predicts a downward dispersion following the cosine function for the transverse branch and upward dispersion for the longitudinal branch, which is exactly what is observed in undoped cuprates. But in $La_{2-2x}Sr_{1+2x}Mn_2O_7$ both branches show a steep downward dispersion above x=0.15. The anomalous dispersion and broadening can be understood as a precursor effect to the CMR transition. This behavior is very unusual, because such precursor effects have previously been associated with phase transitions where charge order appears on cooling, not on heating as in CMR manganites.

MM 26.5 Wed 17:45 H6

Theory of tunneling spectroscopy in UPd_2Al_3 — •David Parker[1] and Peter Thalmeier[2] — [1]MPIPKS, Nothnitzer Str. 38, Dresden 01187 — [2]MPI CPFS, Nothnitzer Str. 40, Dresden 01187

There is still significant debate about the symmetry of the order parameter in the heavy-fermion superconductor UPd_2Al_3, with proposals for $\cos(k_3)$,$\cos(2k_3)$, $\sin(k_3)$, and $e^{i\phi}\sin(k_3)$. Here we analyze the tunneling spectroscopy of this compound and demonstrate that the experimental results by Jourdan et al (Nature **398**, 47 (1999)) are inconsistent with the last two order parameters, which are expected to show zero-bias conductance peaks. We propose a definitive tunneling experiment to distinguish between the first two order parameters.

MM 26.6 Wed 18:00 H6

High-resolution ARUPS on single crystalline FeSi[100] — •M. Klein[1], D. Zur[2], D. Menzel[2], J. Schoenes[2], M. Neef[3], K. Doll[3], G. Zwicknagl[3], and F. Reinert[1] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg — [2]Technische Universität Braunschweig, Institut für Physik der Kondensierten Materie, Mendelssohnstraße 3, 38106 Braunschweig — [3]Technische Universität Braunschweig, Institut für Mathematische Physik, Mendelssohnstraße 3, 38106 Braunschweig

The transition metal compound FeSi shows unique magnetic and transport properties which have been subject to many theoretical proposals but have never been explained completely. To reveal the electronic band structure we have prepared high quality single crystals with a [100] surface and investigated them with high-resolution ARUPS ($\Delta E \sim 3$ meV). Close to the Fermi level we see a narrow band with a small dispersion and a strong temperature dependence. We discuss our results in comparison with band structure calculations and with theoretical models involving narrow bands near the edges of the small gap.

MM 27: HV Kozubski

Time: Thursday 9:30–10:00 Location: H16

Invited Talk MM 27.1 Thu 9:30 H16

Atomic Migration Phenomena in Intermetallics with High Superstructure Stability — •Rafal Kozubski[1], Véronique Pierron-Bohnes[2], and Wolfgang Pfeiler[3] — [1]Interdisciplinary Centre for Materials Modelling, M. Smoluchowski Institute of Physics, H. Jagellonian University, Reymonta 4, 30-059 Krakow, Poland — [2]CNRS, Institut de Physique et Chimie des Matériaux de Straßbourg, CNRS/ULP, 23 rue de Loess BP 43, 67034 Straßbourg, France — [3]Institut für Materialphysik, Universität Wien, Strudlhofgasse 4, 1090 Wien, Austria

Most of the contemporary materials based on intermetallic phases are either multiple bulk phases, or nanostructured layers deposited on appropriate substrates. In each case, the desired properties of the materials are due to chemical order and the preparation technology consists of a generation of specific processes mediated by atomic migration. It is shown how a nanoscopic (atomistic) image of the atomic migration phenomena results from an indirect experimental technique in combination with Monte Carlo (MC) and Molecular Dynamics (MD) simulations.
"Order-order"relaxations were observed in phases representing three typical cubic superstructures of high stability:
$B2(NiAl, FeAl)$, $L1_2(Ni_3Al)$ and $L1_0(FePd, FePt)$.
Detailed analysis of the atomic-jump statistics yielded by MC and MD simulations elucidated: (i) the origin of the multi-time-scale character of the process, (ii) the atomic-jump correlation effect on the effective activation energy for the relaxations, (iv) the effect of free surfaces on the superstructure stability in $L1_0$ nano-layers; (v) the effect of triple-defect formation on the kinetics of the "order-order"relaxation in B2 binaries.

MM 28: Intermetallic phases I

Time: Thursday 10:15–11:15 Location: H16

MM 28.1 Thu 10:15 H16

Empirical effective potentials for complex metallic alloys — •Peter Brommer and Franz Gähler — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Complex metallic alloys (CMAs) comprise materials with promising physical properties. Due to the inherent disorder in these systems, the atomic structure is frequently not reliably known in all details. Atomistic computer simulations are an essential tool both for determining the precise atomic structure and for following the microscopic processes responsible for the macroscopic properties. Unfortunately, first-principles simulations cannot cope with the required system sizes and simulated times, and classical effective potentials are rarely available. We present a programme called *potfit*, which determines the parameters of a classical potential by matching it to a large number of reference quantities computed with first-principles methods. These quantities comprise cohesive energies, stresses and forces on individual atoms in a collection of suitable reference systems. Effective potentials for the MgZn, NbCr, CaCd and AlNiCo systems have successfully been constructed and used in molecular dynamics simulations.

MM 28.2 Thu 10:30 H16

On the thermodynamics of the Pt-Rh alloy: Lattice Monte Carlo simulations using a refined BOS mixing model — •Johan Pohl and Karsten Albe — TU Darmstadt, Fachbereich Material- und Geowissenschaften, Petersenstr. 23, D-64287 Darmstadt

The phase diagram of Pt-Rh printed in most collections of phase diagrams shows a broad miscibility gap. Recent theoretical and experimental studies in contrast indicate that this gap does not exist, but that stable low-temperature ordered phases are present. We calculated the critical temperatures of the theoretically predicted ordered structures and short range order at high temperatures by means of Lattice Monte Carlo simulations using a refined BOS mixing model. This model is able to accurately reproduce the enthalpy of mixing at finite temperatures obtained with the cluster expansion formalism and subsequent cluster variation. Given its simplicity, our model allows computationally more efficient Monte Carlo simulations than the cluster expansion and may also be used for the modelling of nanoparticles. We obtained configurational free energies by thermodynamic integration in the semi-grand canonical ensemble for the different solid solution phases and the implications on phase stability will be presented.

MM 28.3 Thu 10:45 H16

Prediction of stable long-period superstructures in Cu-Pd, Ag-Pd and Au-Pd within a first-principles approach — •Stefan Bärthlein[1], Elke Winning[1], Gus Hart[2], Alex Zunger[3], and Stefan Müller[1] — [1]Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602 — [3]National Renewable Energy Laboratory, Golden, Colorado 80401

One- and two-dimensional long-period superstructures (LPS), based on the $L1_2$ substructure, are systematically investigated for the noble metal-palladium alloys Cu-Pd, Ag-Pd and Au-Pd with first-principles methods. Notwithstanding the fact that the experimental phase diagrams of these systems yield totally different features, quite similar behaviour with respect to formation of low temperature ordered LPS-phases (Cu_3Pd: LPS 3 [1], Ag_3Pd: LPS 3, Au_3Pd: LPS 2; {Cu, Au}Pd_3: $L1_2$, $AgPd_3$: not a ground state) is predicted. As a lever between via LDA obtained formation enthalpies and a thorough ground state scan, the cluster expansion method in conjunction with a genetic algorithm [2] provides adequate means for the extraction of effective interactions, which also allow for an enhanced ground state scan in the configurational space of LPS structures. As a result, the sequences and energetical hierarchies for stable LPSs in Cu-Pd, Ag-Pd and Au-Pd are predicted and compared to conclusions based on an ANNNI-approach. (Supported by DFG.)
[1] Stefan Bärthlein et al., J. Phys.: Fast Track Comm., accepted (2006)
[2] Gus L. W. Hart et al., Nature Materials **4** 391 (2005)

MM 28.4 Thu 11:00 H16

An atomistic view on brittle fracture of complex metallic alloys — •Frohmut Rösch and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Cracks in brittle solids propagate by successively breaking bonds. The fracture behaviour on this atomic level can be mimicked and understood with the help of molecular dynamics simulations. For this purpose we investigate the Friauf-Laves phase C15 $NbCr_2$. The effective potentials for this structurally already quite complex alloy have been matched to ab-initio data for the intermetallic compound. The simulation results reveal that the discreteness of matter strongly effects crack propagation. For this reason major aspects of the computer experiments cannot be explained by continuum theories and global fracture criteria.

MM 29: Intermetallic phases II

Time: Thursday 11:45–13:00 Location: H16

MM 29.1 Thu 11:45 H16

Site occupation and order in γ-TiAl with ternary additions — •Torben Boll[1], Talaat Alkassab[1], Zhi-Guo Liu[2], and Yong Yuan[3] — [1]) Institut fuer Materialphysik der Universitat Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen — [2]) Laboratory of Solid State Microstructures, Nanjing University, Hankou Road 22, Nanjing 210093, China — [3]Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China

Titanium-aluminum-samples with additions of 3at.%Cr, 2at.% Ag and 1-10at.% Nb were prepared by means of levitation melting. The expected dual phase structure of α_2- and γ-phase could be observed with TEM.

The analysis with atom probe tomography (APT) was focused on the $L1_0$-structure of the γ-phase and performed along the superstructure ([001],[110]) and non superstructure ([100]) crystallographic directions.

A new developed algorithm was processed on the APT data to gain information on the site occupation of the ternary additions in the $L1_0$-structure. Results based on statistical evaluation of the data for the different samples will be presented. With this approach it is furthermore possible to attain information about the field evaporation field strengths for the components in the structure, which may differ from the field evaporation field strengths of the pure metals as will be discussed.

MM 29.2 Thu 12:00 H16

First PAC experiments in MAX phases — •Michael Uhrmacher[1], Hans Hofsäss[1], Jens Röder[2], Pawel Wodniecki[3], Agnieszka Kulinska[3], and Michel Barsoum[4] — [1]II. Physikliches Institut, Uni Göttingen, Germany — [2]TU Braunschweig, Braunschweig, Germany — [3]IFJPAN, 31-342 Krakow, Poland — [4]Drexel University, Philadelphia, USA

MAX phases are layered, hexagonal ternary carbides and nitrides which combine some of the best attributes of metals and ceramics: like metals, they are electrically and thermally conductive and most readily machinable. Like ceramics, they are elastically rigid, lightweight and maintain their strength to high temperatures.

PAC experiments with implanted ^{111}In have been performed to establish the PAC signal typical for substitutional probes on the In-site in the two MAX compounds Ti_2InC and Zr_2InC. This determination will be the key to investigate by PAC the microstructure of the full class of MAX phases (about 50 compounds) which do not necessarily contain In ions in the structure. Annealing, thermal stability and first experiments under compresive stress are reported.

MM 29.3 Thu 12:15 H16

Interface Reaction and its Kinetics of Al and Binary Al-alloys on Mild Steel Substrates — •Werner Fragner[1], Roman Sonnleitner[2], Peter Uggowitzer[3], and Jörg Löffler[3] — [1]ARC Leichtmetallkompetenzzentrum Ranshofen GmbH — [2]ECHEM, Kompetenzzentrum f. Angewandte Elektrochemie GmbH — [3]Metal Physics and Technology, Department of Materials, ETH Zurich

To meet the requirements of weight-saving and low-cost production of components for future transport vehicles, the concept of multi-material mix is of increasing importance. In this context aluminum-iron compounds produced by means of compound casting are considered to be of particular importance. An essential and critical aspect of such compound castings is the formation of intermetallic phases (IMP) at the Al-Fe interface. Both the nature and the kinetics of potential IMPs are not well understood and require a systematic investigation. In this presentation we document the interface formation of pure Al and binary Al-alloys on a mild steel substrate by means of isothermal wetting and dipping experiments. Tests were carried out employing the sessile droplet method in a controlled atmosphere and inserting plates into the melt. Using pure Al and Al7Si, Al7Cu, and Al7Zn alloys the interface reactions were investigated by quantitative metallography (LOM, SEM/EDX). Special attention was paid to the influence of the alloying elements on the type and sequence of IMPs at the interface and the kinetics of the interface formation with influences of environmental conditions like surface treatment and additional elements present in the melt.

MM 29.4 Thu 12:30 H16

Non-equilibrium solidification of intermetallic phases in Ni-Al and Ti-Al alloy systems — •Helena Hartmann[1,2], Peter Galenko[2], Hamid Assadi[3], Sven Reutzel[1,2], Roman Lengsdorf[1,2], and Dieter Herlach[2] — [1]Institut für Experimentalphysik IV, Ruhr-Universität, 44780 Bochum, Germany — [2]Institut für Materialphysik im Weltraum, DLR, 51170 Köln, Germany — [3]Tarbiat Modarres University, Tehran, Iran

Rapid solidification of intermetallic alloys can lead to a transition from ordered to disordered growth due to the effect of disorder trapping. It is well known that the kinetics of crystal growth of intermetallic compounds is different from that of disordered solid solutions. In the present work containerless processing by electromagnetic levitation technique is used to measure the dendrite growth velocity as a function of undercooling during the solidification of undercooled Ni-Al (β- and γ'-phase) and Ti-Al (γ-phase) alloy melts of various compositions. The structure and microstructure investigations are performed in order to identify the primary solidified phases. Special attention is payed to investigation of chemically ordered intermetallic phases at the stoichiometric compositions 50:50 and 75:25. The experimental findings are interpreted within current theoretical models for disorder trapping and dendritic growth.

MM 29.5 Thu 12:45 H16

Mechanical milling of single phase beta-Al3Mg2 — •Mira Sakaliyska[1], Sergio Scudino[1], Kumar Babu Surreddi[1], Sebastian Sperling[1], Carsten Thomas[2], Michael Feuerbacher[2], and Jürgen Eckert[1] — [1]IFW Dresden, Institut für Komplexe Materialien, Postfach 27 01 16, D-01171 Dresden, Germany — [2]Forschungzentrum Jülich GmbH, Institut für Festkörperforschung, D-52425 Jülich, Germany

In this work, the effect of mechanical milling on microstructure and thermal stability of the polycrystalline beta-Al3Mg2 phase, a complex metallic alloy (CMA) with a giant unit cell containing about 1168 atoms/u.c., has been investigated. With increasing milling time, the grain size of the beta-phase is reduced from micrometer to nanometer regime. At the same time, the mechanical treatment induces the formation of a nanoscale supersaturated Al(Mg) solid solution. Upon heating, the milled powders display a complex thermal behavior: at low temperatures, the phase evolution during heating is characterized by the rejection of an increasing amount of Mg from the solid solution with increasing temperature. At higher temperatures, a phase which resembles the starting beta-Al3Mg2 phase is formed and no traces of the solid solution can be detected, indicating that the solid solution is metastable and transforms into more stable phase(s). The subsequent exothermic events are characterized by the formation and growth of the beta-Al3Mg2 phase, thus indicating that the formation of the supersaturated solid solution during milling can be reversed by appropriately heat treating the mechanically milled powder.

MM 30: Phase transitions III

Time: Thursday 10:15–11:15 Location: H4

MM 30.1 Thu 10:15 H4

nucleation kinetics analysis of pure liquid Gold * a model case? — •Gerhard Wilde[1] and John Perepezko[2] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany — [2]Department of Materials Science and Engineering, University of Wis-consin-Madison, 1509 University Avenue, Madison 53706, USA

Flux treatments with a molten glass slag are commonly used to promote deep liquid undercooling or even bulk glass formation. Although the technique has demonstrated frequently the capability to yield large under-cooling, the underlying mechanisms remain uncertain. There are sugges-tions of flux induced *nucleant removal* or *surface site deactivation* interactions, but the effectiveness and operation of these processes have not been identified clearly. As a model system, the undercooling response of pure Au encased in Pyrex glass was studied systematically to develop a consistent record of the undercooling behavior. Nucleation kinetics analy-ses of statistically significant sets of measurements performed under strictly controlled conditions reveal the presence of a new mechanism based on gas-solid interactions that trigger nucleation through a nucleant precipitation reaction as the first step of the interaction. A new model, based on thermodynamic considerations and on the nucleation kinetics data is proposed that accounts for the undercooling increase including initial conditioning, atmosphere effects and undercooling saturation in a self-consistent manner.

MM 30.2 Thu 10:30 H4

The effect of melt convection on the secondary dendritic arm spacing of Nd-Fe-B alloys — •Kaushik Biswas[1], Regina Hermann[1], Horst Wendrock[1], Gunter Gerbeth[2], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Forschungszentrum Rossendorf (FZR), Institute of Safety Research, P.O. Box 510119, 01314 Dresden, Germany

Dendritic microstructure is one of the major microstructural constituents of peritectic alloys. In the present work, the effect of melt convection on the secondary dendritic arm spacing (SDAS) and phase fraction of properitectic α-Fe was investigated during solidification of stoichiometric Nd-Fe-B alloys under forced crucible rotation technique. The resulting microstructure of the alloy in consideration of melt convection has been investigated using scanning electron microscopy and optical microscopy. The average SDAS was determined for each sample from the whole cross-section of the cylindrical test samples using image analysing software LEICA QWIN. A detailed statistical analysis of the spacing distribution was performed on the basis of the variation of SDAS values averaged from about 80 to 120 dendrites in different zones. The α-Fe volume fraction measured by vibrating sample magnetometer (VSM) reduces with increasing crucible rotation frequency. Similarly, the SDAS values decrease with increasing rotation frequency. These results are explained from the viewpoint of a reduced melt convection state under steady forced crucible rotation leading to a reduced effective mass transfer coefficient.

MM 30.3 Thu 10:45 H4

Molecular dynamics simulations for calibrating a phase-field model of solidification in Ni-Zr alloys — •Britta Nestler[1], Denis Danilov[1], Hamid Guerdane[2], and Helmar Teichler[2] — [1]Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany — [2]Institut für Materialphysik, Universität Göttingen

Atomic-scale simulations of crystal-melt interfaces in Ni-Zr alloys are performed to determine the energy densities and material parameters for phase-field modelling of solidification microstructures. To set up the phase-field (PF) model, quantities such as the free energy density functions related to the liquidus and solidus lines of the phase diagram, the diffusion coefficients and the interface thickness are calculated from molecular dynamics (MD) simulation data. The kinetic coefficient is approximated by comparing interfacial positions of MD and PF simulations. Direct comparison of PF and MD simulations show a disagreement in the dynamics of the interface motion. To match PF and MD results the diffusion coefficients of the solid and liquid phases in the PF model have been calibrated using a two-sided analytical sharp interface solution. Results of simulated solid-liquid interfaces are presented showing a comparison of concentration profiles across the crystal-melt interface and of the growth dynamics obtained from MD and PF simulations.

MM 30.4 Thu 11:00 H4

Influence of Strain on Phase Transitions in Solids — •Robert Spatschek[1], Efim Brener[1], and Vladimir Marchenko[2] — [1]Institut für Festkörperforschung, Forschungszentrum 52425 Jülich — [2]P.L. Kapitza Institute for Physical Problems, RAS 119334, Kosygina 2, Moscow, Russia

Many magnetic, superconducting and structural phase transitions in solids are accompanied by small lattice distortions which lead 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.

We consider a sharp interface kinetic model of phase transitions accompanied by elastic strain, together with its phase-field realization. Quantitative results for the steady-state growth of a new phase in a strip geometry are obtained and different pattern formation processes in this system are investigated. We consider the case of a dilatational mismatch and a transition in hexagonal crystals involving shear strain as particular applications of this minimum model.

MM 31: Nano structured materials III

Time: Thursday 11:45–12:45 Location: H4

MM 31.1 Thu 11:45 H4

Influence of Grain Size and Porosity on Electrical Conductivity of Nanocrystalline Cerium Dioxide — •Adrian Ferdinand — AG Birringer, Universität des Saarlandes

The influence of grain size and porosity on the transport properties of nanocrystalline, porous cerium dioxide was investigated by impedance spectroscopy. Magnitude and type (ionic vs. electronic) of electrical conductivity of cerium dioxide depends on parameters such as acceptor concentration, oxygen partial pressure of the surrounding gas phase and the grain size in the case of polycrystalline materials. Materials characterised by grain sizes in the nanometer regime and high porosity over the whole sample are interesting for further studies due to their high ratio of surface to overall interface area. Therefore, as a first approach, the influence of grain size and porosity on electrical conductivity was explored. A series of samples was prepared by consolidation and sintering of cerium dioxide nanoparticles with a sufficient variation in the two essential fabrication parameters, i.e. pressure and sintering temperature. Grain size was determined by X-ray diffraction and microscopy methods (REM), porosity by a density measurement based on Archimedes' principle. Furthermore, information on the samples' free surface area could be obtained by nitrogen adsorption measurement. Impedance spectroscopy was used to measure the electrical conductivity. The experimental results are discussed in terms of the space charge model for polycrystalline ionic material.

MM 31.2 Thu 12:00 H4

Tuneable electrical resistance of nanocrystalline platinum — •Martin Sagmeister[1], Ulrich Brossmann[1], Stefan Landgraf[2], and Roland Würschum[1] — [1]Institut für Materialphysik, TU Graz, Petersgasse 16, 8010 Graz, Austria — [2]Institut für Physikalische und Theoretische Chemie, TU Graz, Technikerstrasse 4, 8010 Graz, Austria

Electric field-induced tuning of material properties is usually restricted

to nonmetals such as semiconductors and piezoelectric ceramics. Based on nanocrystalline materials, metals with tunable mechanical [1], magnetic [2], and electronic properties [3] could recently be generated. We show that variations of the electrical resistance of a metal (platinum) in the range of several percent can be reversibly induced at low charging voltages making use of a nanocrystallite-electrolyte composite [3]. Surface charging of the porous nanocrystallite network occurs by the formation of an electro-chemical double layer. The charge-induced resistance variation is analyzed taking into account the modification of the charge carrier density and scattering rate by surface charging. The contribution rising from the charge-induced variation of the lattice constant is found to be small.

[1] J. Weissmüller, R.N. Viswanath, D. Kramer, P. Zimmer, R. Würschum, and H. Gleiter, Science **300** (2003) 312

[2] H. Drings, R.N. Viswanath, D. Kramer, Chr. Lemier, J. Weissmüller, and R. Würschum, Appl. Phys. Lett. **88** (2006) 253103

[3] M. Sagmeister, U. Brossmann, S. Landgraf, and R. Würschum: Phys. Rev. Lett. **96** (2006) 156601

MM 31.3 Thu 12:15 H4

Kinetic properties of internal interfaces in bulk nanostructured materials: radiotracer investigation — •Sergiy Divinski[1], Jens Ribbe[1], Guido Schmitz[1], Juri Estrin[2], Yaron Amouyal[3], Eugen Rabkin[3], and Christian Herzig[1] — [1]Institut für Materialphysik, University of Münster, Münster, Germany — [2]Technische Universität Clausthal, Lehrstuhl für Physikalische Werkstoffkunde, Clausthal-Zellerfeld, Germany — [3]Department of Materials Engineering, Technion - Israel Institute of Technology, Haifa, Israel

Nanostructured materials reveal often hierarchical microstructures. In nanocrystalline Fe-Ni alloy produced by powder metallurgy, the nanosized crystallites were found to be clustered in micrometer-large agglomerates, with grain boundaries between nanocrystallites and interfaces between agglomerates revealing fundamentally different kinetic properties. On the other hand, low-angle and high-angle boundaries typically co-exist in material after a severe plastic deformation procedure. Diffusion investigations in such materials demand a special care. A complete and consistent model of diffusion in such a material was elaborated that allows a systematic experimental investigation of self- and solute diffusion in all possible kinetic regimes.

The radiotracer technique is applied for measuring grain boundary diffusion of Ni and Fe in the nanocrystalline Fe-40Ni alloys produced by powder metallurgy and in nanostructured copper prepared by equal channel angular pressing. Typical boundaries between nanograins were found to reveal diffusivities, which are similar to those in their coarse-grained counterparts. The origin of fast diffusion paths is discussed.

MM 31.4 Thu 12:30 H4

Oxygen diffusion in fully dense nanocrystalline yttria-stabilized zirconia — •Harald Drings[1], Ulrich Brossmann[2], Hans-Eckhardt Schaefer[1], Agnes Szoekefalvi-Nagy[3], Heinz Dieter Carstanjen[3], and Jürgen Fleig[4] — [1]Institut für Theoretische und Angewandte Physik, Univ. Stuttgart — [2]Institut für Materialphysik, TU Graz, Österreich — [3]Max Planck Institut für Metallforschung, Stuttgart — [4]Institut für Chemische Technologien und Analytik, TU Wien, Österreich

It has been recently shown[1] that the oxygen diffusivity in the grain boundaries of n-$ZrO_2 \cdot Y_2O_3$ is strongly enhanced compared to the volume diffusivity. Therefore, nanocrystalline yttria-stabilized zirconia are a most promising material for the application as an oxygen ion conductor in gas sensors or solid oxide fuel cells. The oxygen diffusivity in n-$ZrO_2 \cdot 9.5\,\mathrm{mol\,\%}\, Y_2O_3$ was studied by ^{18}O Tracer diffusion and ERDA. In addition, the Zr diffusivity was studied by ^{95}Zr Tracer diffusion to gain information about the reliability of future n-$ZrO_2 \cdot Y_2O_3$-based devices. The specimens were prepared by gas-phase synthesis of a nanocrystalline metal powder and subsequent oxidation, compaction and sintering using a optimized procedure[2] to obtain fully dense specimens with minimum distance between cracks of more than 500 μm, allowing both tracer diffusion and impedance studies, which is of particular interest within the framework of the Nernst-Einstein relationship.

[1] Knöner et. al., PNAS **100**, 3870 (2003)

[2] Drings et. al., phys. stat. sol. (RRL) **1**,1, R7 (2007)

MM 32: Diffusion and point defects I

Time: Thursday 10:15–11:15 Location: H6

MM 32.1 Thu 10:15 H6

Diffusion of Hydrogen in Amorphous Ceramics of the System Si-B-C-N — •Wolfgang Gruber, Günter Borchardt, and Harald Schmidt — TU Clausthal, Institut für Metallurgie, Thermochemie und Mikrokinetik - AG Materialphysik

Non-oxide ceramics of the system Si-B-C-N have potential applications as high temperature structure materials, surface coatings and dopable semiconductors. Materials produced from polymeric precursors which are transformed into amorphous covalent ceramics by solid state thermolysis are separated in a silicon rich phase and a carbon rich phase. Diffusion of hydrogen plays an important role in the investigation of the mobility and the kind of defects in the amorphous state. Therefore we measured the diffusivities of hydrogen in amorphous ceramics of the system Si-B-C-N with different compositions. For the diffusion measurements we used deuterium as a tracer which was introduced into the samples via isotope exchange from the gas phase. Depth profiling was done with secondary ion mass spectrometry (SIMS). Depending on the composition the diffusion path for hydrogen is the carbon rich phase or the silicon rich phase. A direct interstitial diffusion mechanism accounts for the diffusion of hydrogen in the carbon rich phase and a trap limited diffusion mechanism accounts for the diffusion of hydrogen in the silicon rich phase.

MM 32.2 Thu 10:30 H6

Diffusion-induced recrystallization in thin metal films — •Dietmar Baither, Britta Kruse, Tae Hong Kim, and Guido Schmitz — Westfälische Wilhelms-Universität, Institut für Materialphysik, Wilhelm-Klemm-Strasse 10, D-48159 Münster

Diffusion-induced recrystallization (DIR) was investigated in AuCu and AgPd double layers. The layers were prepared by sputter deposition on glass substrates. In spite of large lattice mismatch of 13.0 % and 5.1 % for the AuCu and AgPd system, respectively, the thin layers grow semi-coherently with (111) texture.

After heat treatment at 708 K or 723 K, various additional intensity maxima occur in the XRD spectra in dependence on the duration of heating. Simulated XRD spectra point out that these maxima cannot be explained by volume diffusion, even if a concentration-dependant diffusion coefficient is supposed. Instead, the existence of new grains with a preferred composition is favoured. Such newly formed grains were found in TEM micrographs of both systems. EDX measurements confirm the transformation of the planar interface into a granular region of distinct composition.

The evolution of the microstructure and the growth of grains with preferred discrete compositions will be described by a thermodynamical model, which considers the elastic stress and its relaxation during recrystallization.

MM 32.3 Thu 10:45 H6

Grain boundary phase transitions in Cu–Bi alloys studied by radiotracer grain boundary diffusion measurements — •Sergiy Divinski[1], Henning Edelhoff[1], Guido Schmitz[1], Christian Herzig[1], and Boris Straumal[2] — [1]Institut für Materialphysik, University of Münster, Münster, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka, Russia

Bismuth addition to copper is known to cause a catostrophic embrittlement of the material. Moreover, strong Bi segregation at copper grain boundaries may result in the formation of a liquid-like layer even in the Cu-rich single-phase region of the corresponding bulk phase diagram [1]. Since the grain boundary diffusion depends very sensitively on the boundary structure, the rate of grain boundary diffusion can serve as a unique probe of phase transitions occurring when alloying Cu with Bi.

In the present investigation, grain boundary diffusion and segregation of Bi in polycrystalline Cu–Bi alloys are investigated by the radiotracer serial sectioning technique using the 207Bi isotope. An observed non-Arrhenius temperature dependence of grain boundary diffusion of

Bi is discussed in relation to the prewetting phase transition at grain boundaries in the Cu–Bi system.

1. S.V. Divinski, M. Lohmann, Chr. Herzig, et al. Phys. Rev. B. 71 (2005) 104.

MM 32.4 Thu 11:00 H6

Ungewöhnliche Diffusion von Ag und Cu in CdTe — •Herbert Wolf[1], Frank Wagner[1], Thomas Wichert[1] und ISOLDE Collaboration[2] — [1]Technische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]CERN, CH-1211 Genf 23, Schweiz

Normale Diffusion äußert sich in einer von der Quelle ausgehenden monotonen Abnahme des Konzentrationsprofils. Im Gegensatz dazu zeigen die Diffusionsprofile von Ag und Cu in den II-VI Halbleitern CdTe, ZnTe und CdZnTe ein völlig anderes Verhalten, wenn die Diffusion unter einem externen Dampfdruck der Metallkomponente durchgeführt wird [1]. So wird in CdTe nach Implantation von ^{111}Ag oder ^{67}Cu und Tempern bei 825 K ein Profil beobachtet, das symmetrisch im Querschnitt des 800 μm dicken Kristall liegt, wobei die ^{111}Ag Konzentration im Zentrum gegenüber den Randschichten fast stufenartig zunimmt und dort 20-fach erhöht ist. Wird hingegen das Diffusionstempern unter externem Te Druck durchgeführt, tritt in den Randbereichen des CdTe Kristalls eine gegenüber dem Kristallinneren stark erhöhte Ag Konzentration auf. Ein quantitatives Modell wird vorgestellt. Dieses Modell berücksichtigt den Einfluss des externen Dampfdrucks während des Temperns und damit die durch die Diffusion intrinsischer Defekte verursachte Änderung der Stöchiometrieabweichung des CdTe Kristalls. Außerdem wird die elektrische Drift geladener Defekte im internen elektrischen Feld, das durch die Konzentrationsprofile der geladenen Defekte verursacht wird, berücksichtigt.

Gefördert durch das BMBF, Projekte 05KK1TSB/7 und CZE 3/002.

[1] H.Wolf *et al.*, Phys. Rev. Lett. 94 (2005) 125901.

MM 33: Diffusion and point defects II

Time: Thursday 11:45–12:45 Location: H6

MM 33.1 Thu 11:45 H6

Thermal vacancies in metallic nanoparticle — •Michael Müller and Karsten Albe — TU Darmstadt. Institut für Materialwissenschaft, FG Materialmodellierung, Petersenstr. 23, D-64287 Darmstadt

The influence of particle size on the concentration of thermal vacancies in metallic nanoparticles is investigated. By analyzing the contributions of surface energies and surface stresses to the vacancy formation energy, a particle size dependent model is derived. The vacancy concentration in metallic nanoparticles is predicted to be smaller than the bulk value. The results are verified by Monte Carlo simulations using a broken bond model and by molecular statics calculations with embedded atom method potentials. The combination of both methods allows to study the influence of surface energies and stresses, separately, and to verify the proposed model description.

MM 33.2 Thu 12:00 H6

Stöchiometrische Leerstellen in Ausscheidungsphasen von Al-Legierungen — •Iris Kohlbach und Torsten Staab — Rheinische Friedrich Wilhelms Universität Bonn, Helmholtz Insitut für Strahlen - und Kernphysik, Nussallee 14-16, 53115 Bonn

Beim Aushärtungsprozess von Aluminiumlegierungen werden Fremdphasen ausgeschieden, die z.T. metastabil sind. Die Legierungen werden lösungsgeglüht und abgeschreckt und die Leerstellen dabei eingefroren. Daraus ergibt sich die Fragestellung ob Abweichungen von der Stöchiometrie in einzelnen Ausscheidungsphasen durch diese Leerstellen kompensiert werden. Dazu wurde für Al-Kupfer-Legierung und AlMgSi-Legierung mit Ab-Initio-Methoden die Leerstellenbildungsenthalpie für die verschiedenen Untergitter, z.B. AL2Cu oder Mg2Si berechnet. Die Berechnungen wurden mit Hilfe des ab-initio Codes SIESTA vorgenommen. SIESTA nutzt hierbei die selbst konsistente Dichtefunktionaltheorie (DFT) für die Berechnung der elektronischen Strukturen. Neben den Leerstellenbildungsenthalpien erhält man bei den Berechnungen mit SIESTA auch die entsprechenden Atompositionen. Die so gewonnenen Atompositionen werden mit experimentellen Ergebnissen aus der Positronenvernichtung verglichen.

MM 33.3 Thu 12:15 H6

Ab-initio modelling of defect properties in B2 NiAl — •Daniel Lerch, Kerrin Dössel, Stefan Müller, and Klaus Heinz — 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 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 elucidate the ordering and ground state properties of defects in B2 NiAl on the basis of ab-initio calculations. We have applied the Cluster-Expansion (CE) formalism with Density Functional Theory (DFT) and the nudged elastic band method (as implemented within the computer code VASP) supplying the required input energies, as well as activation barriers for defect diffusion. Consistent with the existence of vacancies a full description of defects in NiAl bulk is only possible if vacancies are included by treating them as a third independent component within the CE formalism. One possible choice for a complete orthonormal basis set of point functions, required in such a ternary CE, are the first two Chebychev polynomials which were chosen in this case.

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

MM 33.4 Thu 12:30 H6

Ab initio study of the carbon-carbon interaction in iron — •Olga Kim, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The difference in solubility of carbon between the austenite and ferrite is the basis for the solid solution hardening of steels. The C-solubility is determined by the C-C interaction energy that influences the distribution of carbon atoms in both phases. The interaction energy in austenite is easily measurable and well known. However, in ferrite it could not be deduced experimentally due to the very low solubility of carbon in ferrite. In order to gain a detailed insight into this issue we have theoretically determined the dependence of the C-C interaction energy in ferrite as function of the C-C separation by employing density functional theory (DFT) in the generalized gradient approximation (GGA). Our results show that interstitial carbon atoms strongly repel each other. This effect gives rise to the experimentally observed low solubility of carbon in ferrite. The theoretical data provides also direct insight into ordering tendencies of carbon atoms and thermodynamic stability. In a second step the analogous calculations have been performed for austenite. Using these data the temperature dependent carbon activity in austenite is derived and compared to results obtained by the quasi-chemical approximation (R. B. McLellan and W. W. Dunn: J. Phys. Chem. Sol. 30, (1969) 2631) and with available experimental data.

MM 34: HV Lendlein

Time: Thursday 14:00–14:30 Location: H16

Invited Talk MM 34.1 Thu 14:00 H16

Shape-Memory Polymers — •Andreas Lendlein — Institute of Polymer Research, GKSS, Kantstraße 55, 14513 Teltow-Seehof

The ability of polymers to move actively in response to an external stimulus such as heat, light or magnetic field is of high scientific and technological significance. The shape-memory effect as an example for such a functionality will be presented. Upon exposure to an external stimulus, shape-memory polymers have the capability to change their shape in a predefined way. This effect results from the polymer's molecular architecture in combination with a certain processing and programming technology.
Temperature-induced shape-memory polymers are introduced and potential biomedical applications will be described. As light-induced shape-memory polymers are independent of any external heating and do not heat up while irradiated, they especially offer an alternative mode of actuation for medical applications. Moreover, non-contact triggering of shape changes in polymers has been realized by incorporating magnetic nanoparticles in thermally-induced shape-memory polymers. These compounds are heated inductively if they are submitted to alternating magnetic fields.
Each biomedical application is demanding a specific set of macroscopic properties and functionalities (such as degradability). A concept allowing tailoring of properties by varying the molecular parameters and functionalization are polymer systems. The innovation potential of such families of polymers is illustrated for a multifunctionalized material system.

MM 35: SYBM Bioinspired Materials

Time: Thursday 14:45–20:45 Location: H16

MM 35.1 Thu 14:45 H16

Reflection of water jets on biological and bio-inspired artificial surfaces — •Michael Scharnberg[1], Vladimir Zaporojtchenko[1], Rainer Adelung[1], Srdjan Milenkovic[2], and Achim Walter Hassel[2] — [1]Chair for Multicomponent Materials, Technical Faculty, University of Kiel, Germany — [2]Electrochemistry and Corrosion, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Water jets impinging on a nasturtium leaf, a biological ultrahydrophobic surface (lotus effect), were observed to flow across the surface for a distance in the order of several jet diameters before it is reflected off the surface as a coherent jet under an angle that is close to or smaller than the angle of incidence. Design and technical applications of ultrahydrophobic surface require understanding of the physical processes involved, however biological surfaces often have defects and irregularities like leaf veins that impede experiments. A ds-NiAl-W alloy, microstructured by etching and coated with a sputtered polytetrafluoroethylene (PTFE) thin film is also ultrahydrophobic (contact angle $> 160°$). Due to the regular microstructure of its surface that can also be easily varied by controlling the needle length, this ultrahydrophobic material system is well suited for investigation of the water jet reflection phenomenon. In this presentation the influence of the microstructure, the water pressure and the angle of incidence will be discussed.

MM 35.2 Thu 15:00 H16

Enhancement of capillary forces by multiple liquid bridges — •Emerson Jose De Souza[1], Camilla Mohrdieck[2], Martin Brinkmann[3], and Eduard Arzt[4] — [1]Max Planck Institute for Metals Research, Heisenbergstr, 3, Stuttgart, Germany — [2]Institute of Physical Metallurgy, Universität Stuttgart, Stuttgart, Germany — [3]Max Planck Institute for Dynamics and Self-Organisation, Göttingen, Germany — [4]Max Planck Institute for Metals Research, Heisenbergstr, 3, Stuttgart, Germany

Capillary forces can significantly increase the adhesion of micro-scale objects in biology and technology. We calculate numerically the force exerted by a liquid meniscus between two homogeneous flat plates for different contact angles. The resulting force distance curves show good quantitative agreement with previous investigations. On this basis, we set an initial separation and split the volume of one bridge into n smaller ones. The results for the total force as a function of n show a novel and unexpected maximum force for moderately hydrophilic surfaces (i.e. contact angles around 70 degrees). Further, we calculate the minimum area for multiple bridges, the stress (i.e. force per area) and the work required to separate the plates. The results are presented in two dimensional maps, which may be very useful in the understanding and design of biological and artificial contact systems.

MM 35.3 Thu 15:15 H16

Bacterial S-layers used as bio-templates for the regular arrangement of nanoparticles — •Ute Queitsch[1], Elias Mohn[1], Franziska Schäffel[1], Ludwig Schultz[1], Bernd Rellinghaus[1], Anja Blüher[2], and Michael Mertig[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Max Bergmann Center for Materials Research, TU Dresden, D-01069 Dresden, Germany

Owing to the statistical nature of the deposition process nanoparticles from the gas phase are usually randomly distributed on the substrate. For many applications however, a regular arrangement of the particles is mandatory. We have therefore investigated to which degree the use of so-called S-layers – regular protein crystals with different 2-dimensional lattice symmetries – allows to compensate for this disadvantage. S-layers of *bacillus sphaericus NCTC 9602* with p4 symmetry and a square lattice of pores with a lattice constant of 12.5 nm are used as bio-templates for the deposition of gas-phase prepared FePt nanoparticles. Sheets of these S-layers were deposited onto amorphous carbon films, which were then exposed to a beam of FePt nanoparticles under high vacuum conditions. Structural characterization of likewise prepared particle films is carried out by transmission electron microscopy (TEM). We find that the structure of the S-layers remains unaltered upon particle deposition. Furthermore, a symmetry transfer from the bio-template to the arrangement of the deposited particles is clearly observed. Statistical analysis of the TEM micrographs reveals that the majority of the particles are located within or in the close vicinity of the pores of the bio-template.

MM 35.4 Thu 15:30 H16

Inversion of micro-patterned polymer surfaces based on bicomponent polyelectrolyte layers — •Alla Synytska[1], Manfred Stamm[1], Stefan Diez[2], and Leonid Ionov[2] — [1]Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Hohe Strasse 6, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrasse 108, 01307 Dresden, Germany

Micropatterned surfaces are of considerable importance for microelectronics,printing technology, microfluidic and microanalitical devices,information storage, biosensors, etc. However, once a pattern is generated it cannot be easily changed on the fly. Therefore, it is desirable to develop methods for fabrication of structured surfaces with switchable and rewritable patterns.

In the present study, we report on the fabrication of micropatterned surfaces which allow the switching of topography, wettability, and charge in an inverse manner. The concept of these stimuli-responsive surfaces, which are made by a combination of photolithography, liftoff and grafting to techniques, is based on the site-selective grafting of two oppositely charged polyelectrolytes. Depending on the pH of the surrounding one kind of the polymer chains is swollen (charged and hydrophilic) while the other is collapsed (uncharged and hydrophobic). The main advantage of such surfaces is their capability of inverse switching, for example hydrophilic patterns can be reversibly converted into hydrophobic ones and vice versa, via external stimuli.

15 min break

MM 35.5 Thu 16:00 H16

Structure and dynamics of biological materials — •Martin Müller — Institut für Experimentelle und Angewandte Physik, Christian–Albrechts–Universität zu Kiel

Almost all biological materials are hierarchically structured on many different length scales. On a mesoscopic level, usually a composite morphology with nanocrystalline regions embedded in a softer, disordered matrix is found. The matrix is accessible to water, and the water content is of major influence on the mechanical properties of biomaterials.

We investigate structural changes of biomaterials (cellulose fibres, wood and particularly silkworm silk) under mechanical load in *in situ* X–ray scattering experiments with microbeam synchrotron radiation. A novel sample environment allows us to systematically vary the water content of the samples. The soft, water–accessible matrix plays an important role in the microscopic model we obtain for deformation mechanisms in dry and wet biomaterials [1].

The combination of the X–ray results with those from the complementary technique of inelastic neutron scattering allowed us to develop a deeper understanding of the interplay of crystalline and disordered regions in silkworm silk [2].

[1] I. Grotkopp, PhD thesis, Kiel, 2006.
[2] T. Seydel, K. Kölln, I. Krasnov, I. Diddens, N. Hauptmann, G. Helms, M. Ogurreck, S.–G. Kang, M. M. Koza, M. Müller, Macromolecules, in press.

MM 35.6 Thu 16:15 H16

The actuation of organ movement by the generation of tensile and compressive stresses in wood cell walls — •Ingo Burgert, Michaela Eder, Notburga Gierlinger, and Peter Fratzl — Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, 14424 Potsdam, Germany

Active movement is usually associated with animals rather than plants. Plants do not have muscles, but they are able to pre-stress their tissues in order to actuate their organs. Here, we demonstrate for softwoods that either tensile or compressive stresses can be obtained during swelling of the cell wall. This can be well understood by simple mechanical considerations, taking into account the cell shapes and the observed cellulose fibril orientations. The almost inextensible cellulose fibrils redirect the forces generated by the swelling of the matrix by purely geometrical constraints to produce tension or compression forces according to needs. This principle could be simple enough to be reproduced in artificial systems and one may consider developing fiber-reinforced hydrogels as effective microactuators. The main technical challenge would be to reproduce the well controlled fiber orientation found in wood cells.

MM 35.7 Thu 16:30 H16

Bamboo: Mechanical Optimisation and Efficiency — •Ulrike G.K. Wegst[1] and Michael F. Ashby[2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — [2]Cambridge University Engineering Department, Trumpington Street, Cambridge CB2 1PZ, UK

An optimised structure is one which uses the smallest quantity of the best material to perform its function, with adequate safety factor. Structural optimisation occurs not only in mechanical engineering, but also in nature: plants whose stems or stalks approach the optimum shape gain efficiency and a height advantage. Bamboo does this exceptionally. It provides the most efficient material for mechanical performance at minimum mass, supporting large loads due to self-weight and external forces. Bamboo achieves its efficiency in three ways: (i) by using efficient materials such as composites, (ii) by grading the structure, (iii) by shaping the component to form a tube. Investigated here is the material aspect of the structural optimisation of the orthotropic bamboo tube and the role which the microstructure plays in its mechanical performance. Concentrating on the elastic bending behaviour, the stiffness, strength and failure modes of bamboo are reviewed and algorithms and diagrams are proposed which allow the optimum property gradient and section shape to be selected. Man-made materials which exploit all three of bamboo's strategies for mechanical efficiency seem to be very rare. Given the ultimate structural efficiency that this combination allows, developing them in wood-based and other composites, for example, would appear to be worth serious consideration.

MM 35.8 Thu 16:45 H16

Hierarchical ceramics from biomimetic processing of wood — •Oskar Paris, Atul Deshpande, and Ingo Burgert — Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

The processing of plant tissues has been used since hundreds of years to obtain useful materials such as paper and activated carbons. The rich structural hierarchy of plant tissues makes them ideal as scaffolds or casting moulds for the synthesis of hierarchically structured inorganic materials based on carbon or ceramics. Besides potential applications as lightweight nanocomposites for structural applications, such materials are typically porous at several length scales, making them interesting candidates for catalysts and filters. A major challenge in the synthesis process of such materials is to preserve the hierarchical plant structure at all levels while retaining the mechanical integrity. We have used wood tissue as a casting mould for the synthesis of hierarchical mesoporous oxide ceramics with directional porosity on the micrometer and the nanometre scale. In particular, we could demonstrate that the entire structure of the wood tissue including the spiralling microfibrillar orientation of the cellulose fibrils can be transformed into a mesoporous Ce0.5Zr0.5O2 ceramic [1].

[1] A. Deshpande, I. Burgert, O. Paris, Small 2 (2006) 994.

15 min break

MM 35.9 Thu 17:15 H16

TiO2 nanotubes: a bio-inspired and bio-inspiring Material — •Sebastian Bauer[1], Jung Park[2], Klaus von der Mark[2], Eugeniu Balaur[1], and Patrik Schmuki[1] — [1]Department of Materials Science, Friedrich-Alexander-University, Martensstr. 7, 91058 Erlangen. — [2]Department of Experimental Medicine I, Friedrich-Alexander-University, Glückstr. 6, 91054 Erlangen.

Self-organized porous structures have had a high impact in surface science due to the simplicity of fabricating nanostructured surfaces. Particularly highly ordered porous Al and Si have attracted significant scientific interest due to the potential applications in different fields. These structures can be achieved essentially by simple anodization under optimized electrochemical conditions. For Titanium we recently reported the preparation of self-organized nanotubular TiO2 layers on titanium surfaces by anodization in various electrolytes containing fluorides. We showed that tailoring the diameter of the formed nanotubes in a wide range (15 - 100 nm) can be achieved by varying the applied potential of the electrochemical setup. The resulting different nanoscale surfaces can be used to evaluate size effects on biorelevant reactions. We will discuss the wetting behavior of these nanoporous surfaces and show that it can be tailored from super-hydrophilic to super-hydrophobic by variation of tube diameter and by light interactions. Furthermore as titanium and its alloys are mainly used as implant materials it is also of interest to see how tissue reacts to the different nanoscales. To evaluate the influence of tube size, tests with rat mesenchymal stem cells were carried out and will be reported.

MM 35.10 Thu 17:30 H16

Material and structural dynamics in trabecular bone — •R. Weinkamer[1], D. Ruffoni[1], J. Dunlop[1], M. Hartmann[2], Y. Brechet[3], P. Roschger[4], K. Klaushofer[4], and P. Fratzl[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]C.E.A./Saclay, Gif-sur-Yvette, France — [3]LTPCM, ENSEEG, Grenoble, France — [4]Ludwig Boltzmann Institute of Osteology, Vienna, Austria

In trabecular bone different hierarchical levels contribute to its mechanical performance. In our simulation work we focus on the level of the foam-like architecture and on the inhomogeneity of the material bone itself. Two different processes are responsible for the ongoing changes on the structural and material level: the remodeling where small bone packets are continuously resorbed and deposited and the mineralization process where the mineral content increases in a newly deposited bone packet. The renewal of bone material is mechanically controlled, that is bone is deposited preferentially at mechanically highly loaded sites. Since the details of this control are unknown, a computer model with different realizations of the mechanical feedback loop has been employed, to study their influence on architecture and time evolution. With a separate model, the heterogeneous mineral content of bone at the material level was investigated. An increase in the mineral content results in a stiffer, but also more brittle material. Predictions are presented of the evolution of the frequency distribution of mineral content in situations of increased remodeling like in osteoporosis or in therapies which aim at reducing the remodeling.

MM 35.11 Thu 17:45 H16

Influence of structural principles on the mechanics and efficiency of different biological materials using lobster cuticle as a model material — •Christoph Sachs, Helge Fabritius, Svetoslav Nikolov, and Dierk Raabe — Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany

The cuticle of the lobster Homarus americanus is a nano-composite material consisting of a matrix of chitin-protein fibers associated with various amounts of crystalline and amorphous calcium carbonate and is organized hierarchically on all length scales. The chitin protein fibers are arranged in horizontal planes where the long axes of the fibers are all oriented in the same direction. These planes are stacked with the orientation of the fibers in superimposed layers rotating gradually around the normal axis of the cuticle, thus creating a typical twisted plywood structure. Additionally, the fibers are arranged around the cavities originating from the extremely well developed pore canal system of the lobster which gives the structure a honeycomb-like appearance. Tensile, compression and shear tests performed on both cuticle in its natural hydrated and in the dry state show that both structural principles, twisted plywood and honeycomb, are reflected in the obtained mechanical data of the material. The comparison of hard mineralized cuticle and unmineralized joint membranes shows the influence of the incorporation of minerals on the performance of the material, which is optimized for the role the material has to play in the living organism. The obtained mechanical properties are used to deduce general analytical models describing the mechanics of different biological materials.

MM 35.12 Thu 18:00 H16

Recombinantly produced Spider Silk in a Microfluidic Device — •Sebastian Rammensee[1], Ute Slotta[2], David Keerl[2], Thomas Scheibel[2], and Andreas Bausch[1] — [1]Technische Universität München, Physik-Department E22-Biophysik, James-Franck-Strasse 1, 85747 Garching — [2]Technische Universität München, Department Chemie, Lichtenbergstrasse 4, 85747 Garching

Spider Silks are protein materials which show mechanical properties being superior to all man-made materials in regard to toughness and elasticity. However, commercial applications of natural spider silk are complicated by the highly cannibalistic and territorial behavior of spiders. This problem can be circumvented by recombinant production of spider silk analogous proteins in bacteria. In vivo, the highly complex spinning process is performed in a specialized organ, being a topic of current research. We study the process of silk fiber formation in microfluidic devices under laminar flow conditions, where mixing occurs only by diffusion. As we have a whole set of recombinantly produced spider silk analogous proteins available for experiments, the influence of different structural features of the proteins on fiber formation can be studied. We present secondary structure information obtained by infrared spectroscopy and Scanning Electron Microscopy images of the produced silk assemblies. We model the elongational flow in the microfluidic channel by Finite Element Simulations, and thus correlate the structure and mechanical properties of the resulting silk structures with the conditions in the spinning channel.

MM 35.13 Thu 18:15 H16

Tension and geometry determine cell and tissue shape — Ilka Bischofs[1], Dirk Lehnert[2], Franziska Klein[2], Martin Bastmeyer[2], and •Ulrich Schwarz[3] — [1]University of California at Berkeley, Department of Bioengineering, 717 Potter Street, Berkeley CA 94720, USA — [2]University of Karlsruhe, Institute of Zoology I, Haid-und-Neu-Strasse 9, D-76131 Karlsruhe, Germany — [3]University of Heidelberg, Im Neuenheimer Feld 293, D-69120 Heidelberg, Germany

Cells adapt their shape in response to the biochemical and physical properties of their environment. Cell shape in turn can determine cell growth and fate. In order to study cell shape as a function of spatially separated ligand patches, we have cultured cells on a square arrangement of fibronectin dots with a large variety of different dots sizes and lattice constants. We found that in any case, cell shape resembles a sequence of circular arcs composed of actin fibers connecting neighboring sites of adhesion. The same morphology has been observed before on the tissue level, namely for fibroblast-populated collagen gels pinned to a flat substrate. Quantitative image analysis revealed that in both cases, a characteristic relation exists between spanning distance and arc radius which can be explained by a mechanical model which includes the effect of both tension and elasticity. Our results suggest that the same universal principles determine the shape of cells and tissues.

MM 35.14 Thu 18:30 H16

The cytoskeleton as an example of a highly adaptive structure — Florent Dalmas[1,2] and •Camilla Mohrdieck[1,3] — [1]Max Planck Institute for Metals Research, Stuttgart, Germany — [2]Present Address: Laboratoire de Recherche sur les Polymères, CNRS - UMR 7581, 94320 Thiais, France — [3]Inst. for Physical Metallurgy, University of Stuttgart, Germany

The internal polymer network of eukaryotic cells, the cytoskeleton, is a very interesting example of a smart structure that integrates sensors, actuators and control systems to perform many vital cellular functions. It is able to adapt and respond to a large variety of intra and extracellular stimuli efficiently and often also interactively. This agility is largely due to a variety of molecules that bind to cytoskeletal fibers to execute certain functions, e.g. crosslinking the fibers. To mimic the adaptiveness of the cytoskeleton in engineered structures, it is necessary to identify the components that act as sensors or actuators and how they interplay.

To address this complex issue, we have focused on the effect of crosslinking on the mechanical stability and the adaptiveness of the cytoskeleton. In a new modeling approach, we describe the cytoskeletal fibers and the molecules that crosslink them into a three dimensional network as homogeneous straight beams in a constant volume. The response to a mechanical stimulus is simulated by subjecting the network to a homogeneous shear stress and calculating its shear modulus. New scaling behaviors of the shear modulus are found and analysed. They indicate general design principles of adaptive networks.

MM 35.15 Thu 18:45 H16

Biomimetic mineralization: the effect of polystyrenesulfonate on the growth of calcite crystals — •Barbara Aichmayer, Helmut Cölfen, Oskar Paris, and Peter Fratzl — Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

Macromolecules are of crucial importance for the control of size, shape and arrangement of mineral crystals in biological tissues. Pokroy et al. [1] recently showed that organic molecules in biogenic calcite even induce remarkable lattice distortions. Inspired by the concept of biomineralization, we use a soluble polymeric additive to modify the growth of calcite, which is crystallized from calcium chloride solutions using the CO2 vapor diffusion technique. Polystyrenesulfonate (PSS) was previously shown to have a pronounced effect on the morphology of calcite particles, which were found to be composed of ordered nanocrystalline substructures. According to thermogravimetric analysis, the particles contained a significant amount of polymer (3wt%). [2] By complementing these results and electron microscopy studies with X-ray scattering we aim to get a more detailed picture of the structure of the calcite-PSS particles. Using a microfocus beam (micro-focus beamline at BESSY, Berlin and ID13 at ESRF, Grenoble) enables us to study the wide- and small-angle X-ray scattering behavior of single particles. Our findings on lattice spacings, texture and internal structure of the calcite mesocrystals contribute to a better understanding of biological and biomimetic mineralization.

1 B. Pokroy, A.N. Fitch, E. Zolotoyabko, Adv. Mater. 2006, 18, 2363.

2 T. Wang, M. Antonietti, H. Cölfen, Chem. Eur. J. 2006, 12, 5722.

MM 35.16 Thu 18:45 H16

Diatoms - the source of biotribological inspiration for novel 3D MEMS — Ille C. Gebeshuber[1] and •Richard M. Crawford[2] — [1]Institut für Allgemeine Physik, Technische Universität Wien, Wiedner Hauptstrasse 8-10/134, 1040 Wien, Austria & Austrian Center of Competence for Tribology, Viktor Kaplan-Strasse 2, 2700 Wiener Neustadt, Austria — [2]Alfred-Wegener Institute for Polar and Marine Research, Bremerhaven, Germany

Diatoms are single-celled organisms with rigid parts in relative motion at the micrometre scale and below. They produce interlocked hydrated silica structures with high precision. These micromechanical parts have been evolutionarily optimized during the last 150 million years or more. It is suggested that MEMS/NEMS researchers meet with diatomists to discuss future common research attempts regarding biomimetic ideas and approaches for novel and/or improved MEMS and NEMS with optimized tribological properties [1,2].

[1] Gebeshuber I.C. and Crawford R.M. (2006) Micromechanics in biogenic hydrated silica - hinges and interlocking devices in diatoms, Proc. IMechE Part J: J. Eng. Tribol. 220(8), 787-796

[2] Gebeshuber I.C., Stachelberger H. and Drack M. (2005) Diatom bionanotribology - Biological surfaces in relative motion: their design, friction, adhesion, lubrication and wear, J. Nanosci. Nanotechnol. 5(1), 79-87

MM 35.17 Thu 18:45 H16

Investigation of the Orientation Relationship Between α-Chitin and Calcite in Crustacean Cuticle Using Synchrotron x-ray Diffraction — •Ali Al-Sawalmih[1], Helge Fabritius[1], Sang-bong Yi[2], and Dierk Raabe[1] — [1]Max-Planck-Institut f. Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf. — [2]Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld.

Crustacean cuticle contains α-chitin-protein organic fibers associated with crystallites of calcite and considerable amounts of amorphous calcium carbonate (ACC). In this study, x-ray pole figure analysis was performed to investigate the crystallographic texture (preferred orientation) of the crystalline calcite and α-chitin, with respect to their orientation relationship, in edible crab *Cancer pagurus* and american lobster *Homarus americanus* cuticles using synchrotron wide-angle x-ray diffraction (XRD). It was observed that the c-axis of the calcite and the b-axis of the α-chitin are firstly preferentially aligned parallel to each other and secondly oriented along the surface normal. The other axes of the α-chitin and calcite are co-aligned with respect to each other throughout the cuticle plane. The synchrotron x-ray crystallographic texture results gave for the first time a statistical description of the orientation relationship between the organic and inorganic components in arthropod cuticle. This result strongly suggests that the fibrous structure of α-chitin assists the growth of calcite crystals in crustacean cuticle, by functioning directly or indirectly as a template for nucleation and subsequent growth of calcite.

MM 35.18 Thu 18:45 H16

Evaluation of different constitutive models for the mechanical behavior of bone at submicron scale — •Svetoslav Nikolov, Helge Fabritius, Christoph Sachs, and Dierk Raabe — Max-Planck-Institut für Eisenforchung, 40237 Düsseldorf, Germany

Hard biological tissues, such as vertebrate bone, show a complex hierarchical structure at all length scales. The basic structural unit of bone is a fibrous collagen matrix containing small hydroxyapatite crystals in the form of platelets. Here we focus on the constitutive modeling of a bundle of these mineralized collagen fibrils in order to predict their mechanical response. The material is modeled via a two-step homogenization procedure * a first homogenization step at the level of one single mineralized fibril, and a second one at the level of a fibril bundle embedded in an extrafibrillar matrix. We compare different combinations of homogenization models, such as shear-lag models, self-consistent estimates, Mori-Tanaka and double-inclusion homogenization schemes, in order to elucidate which two-step homogenization scheme better reproduce the mechanical data available from experiments. We additionally perform a parametric study on the microstructure parameters, such as the aspect ratio and the volume fraction of collagen fibrils and apatite platelets, the Young*s modulus of the constituents and their density in order to extract some structural optimization principles involved in the natural formation of hard tissues.

MM 35.19 Thu 18:45 H16

Grazing-incidence X-ray scattering investigation on the structure of thin films of recombinant spider silk proteins — •E. Metwalli[1], U. Slotta[2], C. Darko[1], S. Roth[3], T. Scheibel[2], and C. Papadakis[1] — [1]Physikdepartment E13, TU München, 85747 Garching — [2]Chemiedepartment, TU München — [3]HASYLAB at DESY, Hamburg

Protein immobilization on solid supports is important for many potential applications such as protein microarrays. Recombinant spider silk proteins offer the possibility to control the molecular sequence and thus the material properties [1]. Spin-coating was used to prepare films of synthetic spider silk protein derived from the garden spider's (Araneus diadematus) dragline silk protein ADF-4. A transition from alfa-helix to beta-sheet rich structures upon methanol treatment of the films has been detected by IR and circular dichroism spectroscopies [2]. We present here direct evidence for this structural transformation. We have observed crystalline domains within the films after treatment and could determine their size and shape using grazing-incidence X-ray diffraction (GIXD) and small-angle scattering (GISAXS). GIXD showed Bragg peaks from beta-sheet poly-alanine crystallites having a size of 8 nm. GISAXS confirmed the presence of crystallites of this size. We conclude that the protein film structure after the methanol treatment consists mainly of crystalline beta-sheet rich regions embedded in an amorphous matrix. [1] Scheibel T., Current Opinion in Biotechnology 16, 427 (2005). [2] Hummerich D., Slotta U., and Scheibel T., Applied Phys. A-Materials Sci. & Processing 82, 219 (2006).

MM 35.20 Thu 18:45 H16

Structural adaptation in trabecular bone — •John Dunlop[1], Markus Hartmann[2], Yves Bréchet[3], Peter Fratzl[1], and Weinkamer Richard[1] — [1]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Research Campus Golm, 14424, Potsdam, Germany — [2]Service de Chimie Moléculaire, C.E.A./Saclay, Bat. 125, 91191 Gif-sur-Yvette cedex, France — [3]Groupe Physique du Métal, LTPCM/ENSEEG INPG, Domaine Universitaire de Grenoble, 38402 Saint Martin d'Hères, France

The structure of trabecular bone results from the complex interaction between bone producing cells (osteoblast), bone absorbing cells (osteoclasts) and signalling cells (osteocytes), and the performance of the bone matrix itself. One of the important factors that regulates the trabecular architecture is mechanical loading. This can be generalised by the Wolff-Roux law: that is, bone in general is deposited where it is mechanically needed and removed where it is not. Changes in mechanical loading are clearly seen to affect cellular activity and also to modify the resultant bone architecture. The precise details of how cells "feel" a stimulus and exactly how they respond are not known, although there are many suggestions that have been proposed. Computer simulation techniques are ideally suited to testing these theories. In this contribution a 3D lattice model of trabecular bone is presented and used to investigate the link between individual cell response and trabecular architecture through both the "remodelling" and "stimulus" rules.

MM 35.21 Thu 18:45 H16

Creation and Surface-Functionalization of Microcapsules of Recombinant Spider-Silk Protein — •Markus Harasim[1], Teresa Bauer[1], Kevin Hermanson[1], Sebastian Rammensee[1], Thomas Scheibel[2], and Andreas Bausch[1] — [1]Physik Department, E22-Biophysik, Technische Universität München, James-Franck-Str.1, 85747 Garching — [2]Department Chemie, Lehrstuhl für Biotechnologie, Technische Universität München, Lichtenbergstr. 4, 85747 Garching

Micron-size sculpted structures are important for encapsulation and functionalization technologies and as building blocks for larger devices. Here, spherical capsules are created through the self-assembly of recombinant spider-silk at liquid interfaces and in solution. Due to the natural properties of the spider silk the capsules are mechanically strong and biocompatible. These capsules can be formed either in bulk or through microfabrication using microfluidic devices, which allow for the direct control of capsule size and shell thickness. Functionalization of the capsules can also be achieved using common biochemical techniques. Because of the silk's unique properties, this technique potentially offers a convenient approach to the formation of biologically-compatible, easily-functionalizable structures.

MM 35.22 Thu 18:45 H16

Effect of calcium concentration on the structure of casein micelles in thin films — •Ronald Gebhardt[1], Ali Ezzeldin Metwalli[2], Stephan Volkher Roth[3], Wolfgang Doster[2], and Peter Müller-Buschbaum[2] — [1]European Synchrotron Radiation Facility, B.P. 220, F-38043 Grenoble Cedex, France — [2]TU München, Physik Department LS E13, James-Franck-Str.1, 85748 Garching (Germany) — [3]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg (Germany)

Caseins are organized in poly-disperse, roughly spherical aggregates with diameters ranging between 150 and 300 nm. They represent with about 80% the largest protein component in milk. The casein micelle of bovine milk consists of four different phosphor-proteins which can be divided into two groups: the calcium insensitive κ-casein and the calcium sensitive αS1-, αS2- and β-caseins. Casein micelles are the raw material for the production of gelled and flocculated milk products, such as cheese, yogurt and ice-cream. Additionally, casein micelles find a broad application in casein films as adhesives or paint, prepared with solution casting or spray coating techniques.

We have investigated the effect of calcium on the structure of casein micelles in thin films using grazing incidence small angle x-ray scattering (GISAXS) at the BW4 USAXS beamline at HASYLAB/DESY in Hamburg. The GISAXS measurements are complemented with optical microscopy and atomic force microscopy to picture the surface

structure [1].

[1] Müller-Buschbaum P., Gebhardt R., Maurer E., Bauer E., Gehrke R., Doster W. (2006) Biomacromolecules 7, 1773-1780

MM 35.23 Thu 18:45 H16

Hardness anisotropy of crystalline α-chitin: An ab-initio based conformational analysis — •Michal Petrov, Martin Friák, Liverios Lymperakis, Jörg Neugebauer, and Dierk Raabe — Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The α-chitin is one of the most abundant biological materials. The complex structure of α-chitin results in a low-weight and high-strength material, which make it a favorable system for potential bio-inspired functional materials applications. In order to gather a deeper understanding of the mechanical properties of α-chitin, study of the elastic properties of pure single-crystalline α-chitin is crucial. We have therefore explored the atomic structure and the hardness anisotropy of crystalline α-chitin. A challenge in identifying the equilibrium structure of α-chitin is the large size of the unit cell consisting of 108 atoms. In order to resolve this complex structure a series of hierarchical approaches/methods is used: A conformational analysis of chitin is performed using computationally fast empirical potentials and tight binding calculations. Based on the conformational analysis a small number of possible atomic configurations could be identified. These structures have then been used as input for accurate ab-initio calculations in order to derive the ground state atomic geometry and the elastic properties of chitin. Finally based on these results we discuss and explain the strong elastic anisotropy of α-chitin in terms of the interplay between covalent and hydrogen bonds.

MM 35.24 Thu 18:45 H16

Micropatterning of ceramics by ion beam sputtering for dental implants — •Sebastian Wille[1], Bin Yang[2], and Rainer Adelung[1] — [1]Lehrstuhl für Materialverbunde, Technische Fakultät der CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Universitätsklinikum Schleswig-Holstein Campus Kiel, Klinik für Zahnärztliche Prothetik, Propädeutik und Werkstoffkunde, Arnold-Heller-Strasse 16, 24105 Kiel

Due to their attractive esthetics, biocompatibility and mechanical properties, zirconia ceramics are increasingly used for dental implants. But they do not form an osseo-integration due to chemical inertness. In order to improve the osseo-integration of zirconia ceramic implants, a microstructure on the ceramic surface is developed with an ion beam sputter process through a thin film mask which exhibits low sputtering rates. The thin film masks covering ceramic surface are fractured to obtain a microcrack network . After sputtering, the network of cracks is transferred as a network of micro- and submicro channels. With this, relatively high aspect ratios for the microstructures can be obtained. Moreover, by filling the cracks with another material with a high sputter resistance, it is also possible to obtain the inverted network microstructure on zirconia ceramic surface.

MM 35.25 Thu 18:45 H16

Optical and Structural Characterisation of Metallised Oligonucleotides — •Nadine Holzapfel[1], Glenn Burley[2], Johannes Gierlich[2], David Hammond[2], Thomas Carell[2], Gerhard Abstreiter[1], and Ulrich Rant[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — [2]Ludwig-Maximilians-Universität München, Butenandtstr. 5-13, 81377 München

Metallised DNA structures have received considerable attention recently; mainly for their potential applications in nanoelectronic devices. Aside from this, metallised oligonucleotides of nanometer dimensions are expected to exhibit intriguing optical properties due to the excitation of collective oscillations of the conducting electrons by visible light (plasmons). In this study, we used two different methods to deposit silver on oligonucleotides of different lengths (23-96 base pairs). The first method involved the specific labelling of nucleotides with aldehyde groups, followed by exposure to Tollens reagens and a developer, whereas the second method relied on the photoinduced deposition of Ag onto unmodified DNA samples. Several preparation parameters (DNA sequence, buffer salt type, Ag concentration, UV illumination time) were varied systematically. The optical properties of the resulting metallised DNA samples were characterised by recording the extinction spectra using a UV/VIS absorption spectrometer. An extinction maximum was found at ca. 410 nm which is indicative of a plasmonic mode. In addition, the metallised DNA structures were deposited on single crystalline Si wafers and imaged by SEM and AFM.

MM 35.26 Thu 18:45 H16

The rate of bone renewal controls its mechanical behavior — •Davide Ruffoni[1], Peter Fratzl[1], Paul Roschger[2], Klaus Klaushofer[2], and Richard Weinkamer[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Ludwig Boltzmann Institute of Osteology, Vienna, Austria

At the material level bone is a nano-composite consisting of collagen and mineral particles. A crucial factor for the mechanical behavior is the amount and distribution of mineral. Bone material evolves in time as the result of a remodeling and a mineralization process. In trabecular bone the presence of bone packets with different degrees of mineralization is characterized by a bell-shaped frequency distribution of the mineral content, called the bone mineralization density distribution (BMDD). A tailor-made continuity equation is developed to answer how the rate of bone deposition and bone resorption influence the time evolution of the BMDD. First, the steady state solution of the model equation enables the extraction of information on the mineralization kinetics taking the measured BMDD as starting point. Secondly, the knowledge of the mineralization kinetics can be used to predict the full time evolution of the BMDD. Increasing the remodeling rate causes a less mineralized and more heterogeneous mineral distribution. Conversely, when reducing the turnover the BMDD displays transiently a sharp peak corresponding to bone with an unusual uniformity in its mineral content. Later in time higher and less uniform mineralization distributions are attained. From a mechanical view point this suggests an evolution towards stiffer but more brittle bone.

MM 35.27 Thu 18:45 H16

Mechanical properties of silk: Interplay of deformation on macroscopic and molecular length scales — •Imke Diddens[1], Nadine Hauptmann[1], Gesa Helms[1], Igor Krasnov[1], Malte Ogurreck[1], Tilo Seydel[2], Sergio S. Funari[3], and Martin Müller[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian–Albrechts–Universität zu Kiel — [2]Institut Laue–Langevin, Grenoble, France — [3]HASYLAB at DESY, Hamburg

Using an *in situ* combination of tensile tests and X–ray fibre diffraction, we have directly determined the mechanical properties of both the crystalline and the disordered phase of the biological nanocomposite silk. We have adapted a model from linear viscoelastic theory, which fully accounts for the semicrystalline morphology of silk. The elastic moduli of the two phases were determined as well as the relaxing modulus and the viscosity of the disordered matrix. The high extensibility of silk results principally from the disordered phase, however, important elastic deformation was also found in the β–sheet protein crystals. The observed interplay between morphology and mechanical properties will have strong impact on the design of novel protein–based high performance fibres.

MM 35.28 Thu 18:45 H16

Fibrillar level deformation mechanisms in antler — •Stefanie Krauss[1], Himadri Shikhar Gupta[1], Jong Seto[1], John Currey[2], Tomas Landete-Castillejos[3], Sergio Souza Funari[4], Stephan Volkher Roth[4], and Peter Fratzl[1] — [1]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Department of Biology, University of York, York, United Kingdom — [3]IREC (Sec. Albacete) y ETSI Agronomos, IDR, Univ. Castilla-La Mancha, Albacete, Spain — [4]HASYLAB-DESY, Hamburg, Germany

In bone and related biomineralized tissues, the combination of a ductile organic matrix (mostly Type I collagen) with stiff mineral crystallites leads to a material with high stiffness and excellent resistance to fracture. As recently shown by us, the mechanisms leading to this in bone involve shearing in the interfibrillar matrix as well as cooperative deformation between mineral and collagen within the fibril. Deer antler is a less mineralized bone type that shows an extremely high toughness, which has obvious advantages for its physiological function as a weapon during dominance fights between male deer in the rutting period. Using in-situ mechanical testing with time-resolved synchrotron X-ray measurements of the meridional collagen small-angle diffraction pattern, we measured the changes in fibril strain while simultaneously stretching the tissue to failure. We compare the fibril and tissue strain and the variation of the 3rd order meridional collagen peak shape with increasing stress. We discuss how these structural changes at the nanoscale may influence the macroscopic toughness of antler.

MM 36: Nano structured materials IV

Time: Thursday 14:45–16:15 Location: H4

MM 36.1 Thu 14:45 H4

Intrinsic Microstrain in Nanocrystalline Metals — •Jürgen Markmann[1], Vesselin Yamakov[2], and Jörg Weissmüller[1,3] — [1]Universität des Saarlandes, FR 7.3 Technische Physik, 66123 Saarbrücken — [2]National Institute of Aerospace, Hampton, Virginia 23666, USA — [3]Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen

Microstrain is often observed as a consequence of plastic deformation of metals and its appearance is usually contributed to the increase of dislocation density after deformation. Interestingly almost all nanocrystalline metals show already a high amount of microstrain in their as-prepared state independent of their synthesis route. This leads to the assumption that microstrain could be an intrinsic property of nanocrystalline metals. To investigate this, defect-free nanocrystalline 3-dimensional microstructures containing between 16 and 1024 grains were thermally relaxed at 300 K by molecular dynamics simulation. X-ray diffractograms were calculated out of the atom positions and the x-ray peak broadening was analysed to determine the average grain size and microstrain. The evaluated grain size is in excellent agreement with the grain size of the starting microstructure. Nevertheless there is a large the amount of microstrain in the relaxed samples. These findings support an intrinsic nature of microstrain in nanocrystalline metals because no extrinsic sources for microstrain in these "samples" exist. A simple model will be presented which can explain this intrinsic microstrain as a function of the grain size.

MM 36.2 Thu 15:00 H4

The effect of grain size on strain rate sensitivity and activation volume — •Kerstin Schüler, Delphine Lemaire, Thomas Waschkies, Bo Yang, and Horst Vehoff — Werkstoffwissenschaft und Methodik, Universität des Saarlandes, 66123 Saarbrücken, Deutschland

The strain rate sensitivity of nanocrystalline (nc) nickel (Ni) was studied at different temperatures in tensile tests and with a nanoindenter in order to examine the effect of grain size on the different deformation mechanisms of nc materials. The experiments yielded, depending on temperature and strain rate, the strain rate sensitivity, the activation volume and the creep exponents as a function of stress and grain size. From the creep experiments the transition between grain boundary sliding and dislocation climb as a function of temperature was obtained. The strain rate jump tests gave extremely small activation volumes, nearly a factor of 100 smaller than in conventional Ni as a function of grain size. For understanding this behaviour the strain rate sensitivity of single grains was tested with a nanoindenter. The results clearly showed that the primary interaction of dislocations with grain boundaries is the reason for the observed strong rate effects and small activation volumes.

MM 36.3 Thu 15:15 H4

Basic investigations of the precipitation behaviour of AlMgSi alloys — •Ingmar Wieler, Nelia Wanderka, and John Banhart — Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin

AlMgSi alloys are widely used in aerospace applications and in increasing quantity for car body panels. Their beneficial mechanical properties are achieved by precipitation of nanoscaled metastable precursors of Mg_2Si during heat treatment. A room temperature storage after solution heat treatment often results in a slowered and decreased hardening during subsequent artifical aging - the so called negative effect.

Two high purity alloys AlMg0,6Si0,8 and AlMg0,8Si0,6 were produced and subjected to natural as well as artificial aging with and without previous natural aging and a pre-aging step. Certain states have been characterized by hardness and in situ electrical resistivity measurements. Qualitative and quantitative TEM investigations have been made to associate the properties with the microstructural evolution.

The room temperature storage before artificial aging at 180°C gave rise to a distinct delay and reduction of the hardness growth especially for the Si-richer alloy. The resistivity of artificial aged samples was increased by the room temperature storage until about peak hardness was reached. The TEM investigations proved a low-density, coarse precipitate structure to be the reason for the negative effect.

MM 36.4 Thu 15:30 H4

Microstructure Analysis of Al-Mg-Si alloys with respect to its influence on strength — •Cynthia Chang, Nelia Wanderka, and John Banhart — Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin

Al-Mg-Si - based alloys are widely used in automotive industry owing to their high strength, good formability and low density. During paint baking of car bodies at 180°C the metal alloy hardens. The increase of hardness is due to the formation of small needle-like precipitates.

In the present work the influence of different Mg and Si contents is investigated. Alloys with compositions Al-0.4Mg-0.4Si and Al-0.4Mg-1.0Si were characterized after different heat treatments using TEM and microhardness measurements. The strengthening by natural ageing of the both alloys is different. In the case of the Al-0.4Mg-0.4Si alloy the natural aging increases the microhardness after subsequent artificial aging at 180°C, while in case of the Al-0.4Mg-1.0Si alloy it decreases. Preceding natural aging has a positive influence on the strength of Al-0.4Mg-0.4Si and a negative one on Al-0.4Mg-1.0Si alloy.

TEM analysis showed that the small needle-like precipitates of both alloys are oriented parallel to the <001> directions of the Al matrix. While the Al-0.4Mg-0.4Si alloy shows a large number of dislocations beside the needle-like precipitates, no dislocation in the Al-0.4Mg-1.0Si alloy were observed. The number density and the size of needle-like precipitates of both alloys are different too.

The different strengthening behaviour of both materials is discussed with respect to their different microstructure.

MM 36.5 Thu 15:45 H4

Mechanically alloyed nanocrystalline Fe-Cu-powders investigated by Atomprobe Tomography (APT) — •Catharina Wille[1], Taláat Al-Kassab[1], Pyuck-Pa Choi[2], and Reiner Kirchheim[1] — [1]Georg-August-Universität Göttingen, Institut für Materialphysik — [2]Korea Institute of Science and Technology, Nano-Materials Research Center

Atom Probe Tomography (APT) has been applied systematically to characterize mechanically alloyed powders chemically and microstructurally. Such powders are interesting from a technical point of view owing to their outstanding macroscopic properties and their frequent application as feed stock for powder metallurgical processing routes. Fe-Cu serves in this study as a binary model system representative for immiscible systems, characterized by a positive heat of mixing. Powders with concentrations between 2.5 and 10at% Cu were prepared by high energy ball milling applying milling times between 2 and 50h. In addition to the APT, Field-Ion-Microscopy- (FIM) and X-Ray-Diffractometry (XRD) -investigations are performed as well. Thus detailed nanoscale information on the local concentration of the minority component, segregation effects and the distribution of impurities can be gained. In this contribution results on the extension of the solubility limits and on the homogeneity of the alloy - both in dependency on the composition and milling time - are presented, discussed and compared to earlier works. Financial support from the Deutsche Forschungsgesellschaft under contract KI-230/33-1 is gratefully acknowledged.

MM 36.6 Thu 16:00 H4

Microstructural investigations of the carbon free stainless maraging steel Corrax — •Stefan Höring, Nelia Wanderka, and John Banhart — Hahn-Meitner-Institute Berlin, Glienicker Str. 100, 14109 Berlin

Stainless maraging steels are highly alloyed precipitation hardened martensitic steels. Glass and plastic press-forming is one potential application due to their good combination of high toughness and high ductility and the absence of carbides. Precipitates of nanometre size are the reason for the high hardness of these steels. The hardening phase of the commercial alloy Corrax was chemical analysed using the 3D atom probe. The investigation after different aging times at 475°C show only one type of precipitates enriched in Ni and Al. They grow from spherical shaped particles with a size of about 3nm to plates with increasing aging times. The crystallographic structure of these precipitates was investigated with TEM/SAED. These measurements

showed an ordered B2-structure. The changes in the microstructure during aging was analysed by X-ray diffraction. The content of reverted austenite in Corrax which influences the mechanical stability was analysed with diffraction methods after different heat treatments. The results are discussed with respect of the mechanical properties.

MM 37: Nano structured materials V

Time: Thursday 16:45–18:00 Location: H4

MM 37.1 Thu 16:45 H4

Assembly of shape controlled nanocrystals at nanopatterned interfaces — •Eva Bock[1,2], Angela Fiore[3], Liberato Manna[3], and Joachim Spatz[1,2] — [1]Max-Planck-Institute for Metals Research, Dept. New Materials & Biosystems, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]University of Heidelberg, Dept. Biophysical Chemistry, INF 253, 69120 Heidelberg, Germany — [3]National Nanotechnology Laboratories of CNR, Via Arnesano, 73100 Lecce, Italy

Gold nanoclusters with diameters between 2 and 30 nm and lateral distances of 20 to 250 nm are arranged onto silicon or glass substrates with a uniform diameter and a defined interparticle spacing. The patterning technique is based on self-assembly of metal loaded diblockcopolymer micelles (poly[styrene-b-2-vinylpyridine(HAuCl4)]) which form a quasi-hexagonal close packed monolayer. The individual gold nanoparticles are potential candidates for immobilizing single molecules or nanoscopic objects. We developed different methods for the assembly of several nanoparticles on nanostructured surfaces. Nanocrystals of different shape and dimensions have been widely developed during the last decade due to their size- and shape-dependent optical, physical and magnetic properties. One method for the assembly of the nanoparticles is based on thiol-chemistry, the other is based on the hybridization of DNA-strands. For the second way the nanocrystals had first to be transferred from organic into aqueous solution.

This work describes an approach which allows for hierarchical organization of different nanocrystals at interfaces which in turn will allow for tuning its optical properties.

MM 37.2 Thu 17:00 H4

Functional surface nanostructures with highly-regular patterns, tunable properties and broad application potential — •Yong Lei and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Using a new surface nano-patterning technique - the UTAM (ultra-thin alumina mask) nano-patterning, ordered arrays of zero-dimensional nanostructures (such as e.g. CdSe nanodots or Si nanoholes) and one-dimensional nanostructures (such as e.g. carbon nanotubes or Ni nanowires) were fabricated on flat substrates. The ordered nanoparticles and nanoholes were prepared using vacuum evaporation processes and focused-ion-beam etching, respectively. The carbon nanotube arrays were initiated from UTAM-prepared catalyst (metal) nanoparticle arrays in a PECVD process. The feature size of the UTAM-fabricated surface nanostructures can be adjusted in the range of about 10-200 nm. The advantages of the UTAM surface nano-patterning, such as the achievement of tunable properties, large pattern area, high throughput and low equipment costs, make the technique quite suitable to fabricate ordered surface nanostructures with a broad range of potential applications ranging from optics and electronics applications to fabricating nanoscale devices. 1. Y. Lei, et al., Chem. Mater. 17, 580 (2005). 2. Y. Lei, W. K. Chim, H. P. Sun, G. Wilde, Appl. Phys. Lett. 86, 103106 (2005). 3. Y. Lei, et al., Nanotechnology 16, 1892 (2005). 4. G. Wilde, Surface and Interface Analysis 38, 1047 (2006). 5. Y. Lei, W. P. Cai, G. Wilde, Prog. Mater. Sci., in press (2007).

MM 37.3 Thu 17:15 H4

Energy transfer via mechanical and thermal channels in metallic nano-objects arrays — •F Banfi[1], B Revaz[2], C Giannetti[2], G Ferrini[2], P Vavassori[3], V Metlushko[4], M Montagnese[2], F Cilento[2], G Coslovich[5], and F Parmigiani[5] — [1]Department of Condensed Matter Physics, University of Genève, Switzerland — [2]Dipartimento di Matematica e Fisica, Università Cattolica, Brescia, Italy — [3]Dipartimento di Fisica, Università di Ferrara, Italy — [4]Department of Electrical and Computer Engineering, University of Illinois at Chicago, IL — [5]Dipartimento di Fisica, Università degli Studi di Trieste, Italy

2D periodic arrays of permalloy nanodisks deposited on Si substrates are investigated with pump probe optical technique. The 150 fs pump beam (λ=800nm, repetition rate 80 MHz) is used as the excitation source, while the relaxation of the sample is measured recording the variation of intensity of the reflected probe beam as a function of the delay between the pump and probe pulses. The reflected intensity of the first-order diffracted beam is measured. The data show 1) a relaxation of the intensity with a time constant $\tau \sim$ ns 2) oscillations dominated by a frequency $\omega_0/2\pi$ in the GHz range with a damping rate γ. The energy is transfered from the nanodisk to the Si substrate both via thermal and mechanical energy fluxes, the measured time constant τ setting the timescale for these processes. Numerical simulations suggest that the contribution of the two energy channels to the relaxation time can be disentangle. This technique is therefore suitable to measure the specific heat of mesoscopic samples.

MM 37.4 Thu 17:30 H4

Nanoscale ablation induced by laser near-field — •Anton Plech[1], Vassilios Kotaidis[1], Maciej Lorenc[2], Konstantin Istomin[1], and Johannes Boneberg[1] — [1]Fachbereich Physik, Uni Konstanz, Universitätsstr. 10, D-78457 Konstanz — [2]ESRF, BP 220, F-38043 Grenoble; present address: GMCM, Universite Rennes 1, Bat. 11A, Campus Beaulieu, F-35042 Rennes

Experiments on femtosecond laser excited gold nanoparticles are presented and it is shown, that the structure formation of the particles is induced by a non-thermal ablation process, which is induced by the strong local enhancement of the laser field close to the particle surface [1]. Time-resolved x-ray scattering allowed to discriminate the structural manifestations of the excitation process, such as particle heating, melting and relaxation with the environment [2].

[1] A. Plech, V. Kotaidis, M. Lorenc, J. Boneberg: Femtosecond laser near-field ablation from gold nanoparticles, Nature Phys. 2 (2006) 44.

[2] V. Kotaidis, C. Dahmen, G. von Plessen, F. Springer, A. Plech: Excitation of nanoscale vapor bubbles at the surface of gold nanoparticles in water, J. Chem. Phys., 124, (2006) 184702.

MM 37.5 Thu 17:45 H4

SAXS charakterization of silver nanoparticles in glass — •Michael Leitner[1], Gerhard Seifert[2], Bogdan Sepiol[1], and Andrei Stalmashonak[2] — [1]Fakultät für Physik, Universität Wien, Strudlhofgasse 4, 1090 Wien — [2]Institut für Physik, Optik, Martin-Luther-Universitat Halle-Wittenberg, Hoher Weg 8, Halle (Saale)

Glass samples containing silver nanoparticles are of great interest to the optical community because of their special optical properties caused by surface plasmon resonance, resulting in absorption of characteristic wavelengths. Initially spherical particles of about 30 nm diameter can be transformed to ellipsoids by femtosecond laser irradiation in the visible range, which results in optical dichroism of the sample [1]. This method allows the production of high-temperature polarisators.

Here we present SAXS-measurements on the nanoparticles' size distribution and the shape perpendicular to the surface of the sample. The process of interest is as follows: the axis parallel to the polarisation of the laser and elongated at comparably low intensities of the laser shortens at high intensities. Moreover, we can validate the existence and the shape of holes in the matrix created by the dissolution of nanoparticles by a DC field. After the dissolution process no characteristic absorption is detectable any longer and the shape validation by optical means is impossible.

[1] M. Kaempfe, G. Seifert, K.-J. Berg, H. Hofmeister, H. Graener, Eur. Phys. J. D 16, 237-240 (2001)

MM 38: Diffusion and point defects III

Time: Thursday 14:45–15:45 Location: H6

MM 38.1 Thu 14:45 H6

Diffusion of Fe in intermetallic thin films — •Marcus Rennhofer[1], Daniel Kmiec[1], Bogdan Sepiol[1], Gero Vogl[1], André Vantomme[2], Johan Meersschaut[2], Bart Laenens[2], Daniel Merkel[3], Laszlo Bottyan[3], Svetoslav Stankov[4], and Rudolf Rüffer[4] — [1]Fakultät für Physik, Universität Wien — [2]Instituut voor Kern- en Stralingsfysica and INPAC, K.U.Leuven — [3]KFKI, Department of Nuclear Physics, Budapest — [4]ESRF, Grenoble, Cedex, France

Diffusion studies on the mesoscopic and macroscopic scale were done up to now via radio-tracer technique for a wide range of diffusivities. Nevertheless, the resolution of diffusion depths is limited by the detector efficiencies and sputtering resolving power. On the other hand scattering methods with atomic resolution [1] have very limited range of accessible diffusion coefficients. We advantageously applied grazing incidence nuclear resonant scattering of synchrotron radiation [2] for the study of iron self-diffusion in thin intermetallic films of $L1_0$-FePt, $L1_0$-FePd and B2-FeSi. It is possible to measure very low rates of diffusion of about $10^{-21}\,m^2s^{-1}$ to $10^{-25}\,m^2s^{-1}$. We will give a short introduction to the method, and present recent results.

[1] G. Vogl and B. Sepiol, eds. Heitjans and Kärger Diffusion in condensed matter, Springer, *p* 65 (2005).
[2] M. Gupta, A. Gupta, J. Stahn, M. Horisberger, T. Gutberlet and P. Allenspach in Phys. Rev. B 70, 184206 (2004).

MM 38.2 Thu 15:00 H6

How to Measure Diffusion Lengths in the Sub-nanometer Range? — •Harald Schmidt[1,2], Thomas Gutberlet[2], and Michael Bruns[3] — [1]Institut für Metallurgie, AG Materialphysik, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld — [2]Laboratorium für Neutronstreuung, ETH Zürich und Paul Scherrer Institut, 5232 Villigen, Schweiz — [3]Institut für Materialforschung III, Forschungszentrum Karlsruhe, 76021 Karlsruhe

The study of self-diffusion in metastable solids like glasses or nanomaterials necessitates the detection of extremely short diffusion lengths in order to prevent crystallization or growth processes during the measurement. This is especially true for covalently bound amorphous materials with their low atomic mobility. We demonstrate that it is possible to detect diffusion lengths down to 70 Å by neutron reflectometry. Such small values cannot be achieved by conventional methods of diffusivity determination (radiotracer technique, SIMS, NMR, QENS). The reflectivity measurements were carried out on magnetron sputtered amorphous $Si^{14}N_x/Si^{15}N_x$ isotope multilayers which were used as a model system. Due to the periodically modulated structure of the multilayers and the different neutron scattering lengths of the nitrogen isotopes, Bragg peaks occur in the reflectivity pattern. Self-diffusivities down to 5 x $10^{-25}m^2/s$ were determined from the decay of the Bragg peaks due to interdiffusion of the two nitrogen isotopes. The ability of the method to resolve a time dependence of the diffusivities due to short-time structural relaxation is demonstrated.

MM 38.3 Thu 15:15 H6

Eigenschaften struktureller Leerstellen in Fe_3C — •Volker Sluka und Torsten Staab — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelmsuniversität Bonn, Nussallee 14-16, 53115 Bonn, Germany

Eine Methode zur Untersuchung von Ermüdungserscheinungen in Materialien ist die Positronenannihilationsspektroskopie. Die Positronen reagieren dabei empfindlich auf leerstellenartige Kristallbaufehler. Um die Positronensignale aus reinen Kohlenstoffstählen besser zu verstehen, werden ab-initio Rechnungen mit dem SIESTA-Code durchgeführt. Ein solcher Stahl ist ein Gefüge aus einer Ferrit- und einer Perlitphase, wobei Letztere wieder aus Ferrit und Zementit (Fe_3C) besteht. Zunächst werden die Bildungsenthalpien von Leerstellen auf den einzelnen Untergittern des Zementits berechnet. Dabei erhält man die Positionen der um diese Defekte relaxierten Atome. Diese Daten lassen die Berechnung von Positronenannihilationsparametern zu, die dann mit dem Experiment verglichen werden können.

MM 38.4 Thu 15:30 H6

Element specific defect investigation on Mg-alloys by ion implantation with coincident Doppler broadening spectroscopy — •Martin Stadlbauer[1], Christoph Hugenschmidt[2], and Klaus Schreckenbach[1] — [1]TU Munich, ZWE FRM-II, Garching, Germany — [2]TU Munich, Department of Physics E21, Garching, Germany

Magnesium alloys experience an increasing interest for industrial applications due to their low specific weight, high elasticity and mechanical strength. For the high performance of these materials a homogeneous distribution of the alloy constituents is required. It is therefore of great interest to investigate the behaviour of the alloy constituents in the vicinity of open volume defects.

In order to investigate the influence of defects and their chemical surrounding, polished and annealed samples of pure magnesium and the alloy AZ31 (3 wt. % Al and 1 wt. % Zn) were irradiated with Zn-, Al- and Mg-ions. The energy of the ions was chosen between 1.4 MeV and 3.0 MeV according to 2.3 μm mean implantation depth. For every type of material a set of 4 samples was produced with doses between $3 \cdot 10^{13}$ and $3 \cdot 10^{16}\,cm^{-2}$. First, Doppler-Broadening measurements as a function of the positron implantation energy as well as lateral position with a resolution of 2 mm were recorded in order to image the ion beam spot on the sample. Secondly, coincident Doppler-broadening spectra were measured at different positron penetration depths according to the Makhov-profile. The relation between elemental signature and defect concentration in the sample are discussed.

MM 39: Mechanical properties I

Time: Thursday 16:15–18:15 Location: H6

MM 39.1 Thu 16:15 H6

Tribological performance of WC/C coatings on rough substrates — •Mikhail Kosinskiy[1], Yonghe Liu[1], Maik Gubisch[2], Lothar Spiess[2], and Juergen A. Schaefer[1] — [1]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany — [2]Institut für Werkstofftechnik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

The available measurements on the tribological behavior of WC/C multilayer coatings are mainly performed on atomically smooth Si surfaces. In this work, we study the influence of surface roughness on the friction and wear of WC/C coatings. Chromium steel samples cut from linear bearing were polished to surface roughness (Ra) in the range of 3 nm ˜ 700 nm, and subsequently deposited with 700 nm thick WC/C coatings. The measurements were performed by using a reciprocating microtribometer at different normal load and velocity in normal atmospheric conditions. As a comparison, bare samples (without coating) were also tested. We find a roughness, on which the coefficient of friction (COF) is minimum for bare samples, but is maximum for coated samples. The reduction of COF by applying the coating is ˜200%.

MM 39.2 Thu 16:30 H6

Evaluating creep behaviour of thin wall structures at high temperatures - method and first results — •Rainer Hüttner, Rainer Völkl, and Uwe Glatzel — Rainer Hüttner, Metals and Alloys, University of Bayreuth, Ludwig-Thoma-Straße 36b, D-95447 Bayreuth, Germany

The knowledge of creep behaviour of structural materials for high temperature applications is prerequisite for life-time predictions. In order to optimize both the cooling efficiency and the weight of fast rotating turbine blades a general trend to reduce the wall thicknesses of the hollow investment castings is observed. This work deals with a method for evaluating creep behaviour of thin wall structures. The test equipment uses resistive heating to achieve fast heating and cool-

ing rates. The environment during testing can be changed to vacuum, inert gas or air in order to determine in-situ oxidation effects on creep behaviour. Creep strain is measured with accuracy better than 0.1% by a non-contacting image vision technique. A video extensometer and the software SuperCreep is used to reach this high resolution. The principles of this technique and first results will be presented.

MM 39.3 Thu 16:45 H6

Atomistic simulations of the dislocation motion in Fe with solute atoms — •Christopher Kohler and Siegfried Schmauder — Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre, Universität Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany

Solute atoms in metals lead to a strengthening effect by impeding the motion of dislocations. This results from a short-range interaction of the solutes with the dislocation cores as well as from a long-range interaction of a distribution of many solutes with the dislocations. Molecular dynamics (MD) simulations with empirical interatomic potentials, e.g. EAM potentials, are a suitable method to model the dislocation-solute interaction at the atomic scale. In this talk, results of MD simulations of solid-solution strengthening in α-Fe are presented. The gliding of dislocations under the influence of an applied shear stress and at different temperatures is studied for random distributions and specific configurations of solute atoms. The effect of solute atmospheres around the dislocation core is also investigated.

MM 39.4 Thu 17:00 H6

Local stress incompatibilities as source of dislocation nucleation and damage — •Markus Welsch, Michael Marx, and Horst Vehoff — Universität des Saarlandes, Werkstoffwissenschaft und Methodik, Postfach 15 11 50, 66041 Saarbrücken, Deutschland

During high cycle fatigue of polycrystalline materials local inhomogeneities cause localized additional stresses. For instance due to elastic anisotropy orientation differences at grain boundaries work as additional driving forces for damage mechanisms. This was shown by experiments and simulations in a previous work, where cracks initiated exactly at grain boundaries with the highest incompatibility stresses calculated by finite element method (FEM). In the further work these experiments are extended to local plastic deformation at higher loads. The stress distribution of an elastic anisotropic material is calculated by FEM. This calculation uses the 3-dimensional arrangement of the grain boundaries and the orientation of the grains determined by electron backscatter diffraction. In the range of beginning elastic-plastic deformation, the local additional stresses are absorbed by the formation of dislocation structures (DS). DS and persistent slip bands develop, which also act as preferential crack initiation sites. These DS are examined by electron channelling contrast imaging. During fatigue in the grains of different orientation strongly varying DS are formed. But also inside these grains the arrangement of the structures is not uniform. Near grain boundaries seams with different DS are generated. The influence of incompatibility stresses on DS and their influence on crack initiation and propagation are presented in this work.

MM 39.5 Thu 17:15 H6

Simulation der Materialermüdung durch einen neuen, granularen Ansatz — •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

In einem neuen Ansatz wird die Ermüdung eines Metalls mit einem granularen, mesoskopischen Modell simuliert. Der Kristall wird als regelmäßige Anordnung von Kristallkörnern betrachtet, deren in der Realität sehr komplexe Eigenschaften auf einige wenige skalare Parameter reduziert werden: Korngröße, Orientierung und E-Modul. Die sich während der Ermüdung erhöhende Versetzungsdichte wird dabei durch einen Schädigungsparameter repräsentiert. Informationen über die Schädigung werden durch lokale Übergangsfunktionen übertragen. In einer ersten Implementierung wird das Verhalten von Nickel im einachsigen Zug-Druck-Versuch schon teilweise wiedergegeben.

MM 39.6 Thu 17:30 H6

Artificial crack initiation and investigation by focused ion beam microscopy — •Wolfgang Schäf, Michael Marx, and Horst Vehoff — Universität des Saarlandes, Werkstoffwissenschaft und Methodik, Postfach 151150, D 66041 Saarbrücken

The influence of the microstructure on fatigue crack growth is of interest in respect to increasing the lifetime of construction materials. A method to investigate the interaction of grain boundaries with short cracks is to introduce micro notches by Focused Ion Beam (FIB) milling in a given distance to a grain boundary. During cyclical loading, a microcrack initiates at the notch tips. The interaction between crack and grain boundary can be studied by measuring the crack velocity in respect to the distance from the grain boundary. A three dimensional tomography of the crack plane and the grain boundary can be revealed by FIB tomography with a resolution comparable to a scanning electron microscope. By this technique, it is possible to visualize the crack plane twist and tilt at a grain boundary. Further, the influence of carbide precipitates on crack growth in a nickel based superalloy was examined. It is shown that this method can also be applied to pure nickel and duplex stainless steel.

MM 39.7 Thu 17:45 H6

Change of deformation mechanism in sub-microcrystalline PED nickel during cyclic loading — •Lutz Hollang[1], Ellen Hieckmann[2], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden — [2]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden

Sub-microcrystalline (smc) nickel produced by pulsed electrodeposition (PED) was cyclically deformed at room temperature at different plastic strain amplitudes $10^{-4} \leq \epsilon_{\mathrm{pa}} \leq 10^{-2}$. The standard plastic strain rate $\dot{\epsilon}_{\mathrm{p}} = 2 \cdot 10^{-5} s^{-1}$ was repeatedly varied to determine the derivative $(\partial\sigma_{\mathrm{a}}/\partial \ln \dot{\epsilon}_{\mathrm{p}})_T$ as a function of the stress amplitude σ_{a}. Both, σ_{a} and $(\partial\sigma_{\mathrm{a}}/\partial \ln \dot{\epsilon}_{\mathrm{p}})_T$ are rather high in the as-prepared state, but significantly decrease during cycling at constant $\epsilon_{\mathrm{pa}} \geq 2.5 \cdot 10^{-4}$ until the specimens exhibit strain localization leading to fracture. X-ray diffraction and transmission electron microscopy reveal that the smc PED nickel cannot resist to ongoing cyclic deformation at room temperature. Already at relatively small ϵ_{pa} dynamic recovery and grain growth processes substantially diminish the internal stresses and transform the as-prepared smc microstructure into a recovered microcrystalline state. The $(\partial\sigma_{\mathrm{a}}/\partial \ln \dot{\epsilon}_{\mathrm{p}})_T$ vs. σ_{a} relationship indicates a gradual change of the rate-controlling process from dislocation–grain boundary interaction at the beginning of cyclic deformation to classical dislocation–dislocation interaction immediately before fracture.

MM 39.8 Thu 18:00 H6

Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS -ICP-MS) in the high resolution study of trace elements distribution patters in selected materials — Watling John[1] and •Chaudhri . Anwar[2] — [1]Centre for Forensic Sciences, Uni. of Western Australia, Perth — [2]Klinikum Nürnberg-Süd, 90471 Nürnberg

One of the major problems for identifying the chemical reasons for fracture or failure of metals and metal alloys is the lack of accurate chemical data for metal concentrations across the failure site. Most modern analytical techniques require the use of relatively large sample masses to ensure accurate multi-element data. The fact that large samples have to be taken often means that there is a significant contamination of the relevant sample with material spatially associated with, but not causative in, the failure. This fact excludes the use of chemical analytical techniques to ascertain the causes of any failure. Techniques such as Scanning Electron Microscopy coupled with Energy Dispersive X-ray Analysis (SEM - EDXRA) can provide micron resolution analytical data. However, the detection limit of the technique is large and as such may not be sufficiently sensitive to identify the true cause of failure. Detection limits of LA-ICP-MS, an analytical technique making use of laser light to ablate a solid sample matrix, are in the sub parts per million level.To illustriate the usefulness of the technique some examples of elemental distributions in different materials are presented.

MM 40: HV Haaks

Time: Friday 10:15–10:45 Location: H16

Invited Talk MM 40.1 Fri 10:15 H16

Material science with positrons: From Doppler-Spectroscopy to Failure Prediction — •Matz Haaks — Helmholtz-Institut für Strahlen und Kernphysik, Nußallee 14-16, 53115 Bonn

Failure of construction parts due to fatigue is a phenomenon well known in everydays life. Since almost 150 years the lifetime of construction parts is determined employing destructive test series like the Wöhler-test, where a huge number of identical samples has to be tested in a very time-consuming way. Up to the present these methods have not changed in principle.

On a microscopic scale material fatigue is based on accumulation of dislocations and other defects in the lattice. Already in the early stages of fatigue - within the first couple of load cycles - a significant increase of the defect density can be observed non-destructively by Positron Annihilation Spectroscopy (PAS) with an extreme sensitivity. Scanning Positron Microscopy (SPM) expands the capabilities of PAS into the micron range. With SPM - employing an annihilation line shape parameter quantifying the Doppler shift due to the electrons momentum (S-parameter) - the density of defects (vacancies, dislocation jogs, vacancy-clusters) in the subsurface layer can be visualised.

Since the density of defects rises during fatigue, it can be employed as a precursor for the final state of failure. Assuming that failure occurs when a critical defect density is reached locally, failure can be predicted from measurements supported by garnular model calculations in the very beginning of fatigue tests.

MM 41: Materials design I

Time: Friday 11:00–12:00 Location: H16

MM 41.1 Fri 11:00 H16

A texture component model for predicting recrystallization textures — •Abhijit Brahme, Myrjam Winning, and Dierk Raabe — Max Planck Institute for steel Research, Max-Planck Str. 1 Duesseldorf 40237

We present an analytical model for predicting crystallographic textures and the final grain size during primary static recrystallization of metals using texture components. The model uses a subset of texture components instead of using the entire set of orientations needed to represent the material. The recrystallization kinetics and the texture evolution are governed by the tensorial variant of the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation. The number of components determines the order of this tensor. Each entry in the tensors represents coupling between the recrystallizing and the deformed components. The growth of a recrystallizing component in to a given deformed component is dependent on various factors like activation energy of nucleation, activation energy for boundary mobility and stored energy (in the deformed region). Main aim of this work is to present a fast and physically based process for simulation of recrystallization texture with respect to processing. We also present preliminary results of application of this method to low carbon steels.

MM 41.2 Fri 11:15 H16

Ab initio calculation of free energies and thermodynamic properties of fcc metals — •Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

Phase diagrams are indispensable tools in predicting material evolution during its processing. Current approaches to obtain such phase diagrams (e.g. CALPHAD) are based on an extra- and/or interpolation of experimental data. A crucial issue hampering this approach is the lack/high cost of specific experimental data (e.g. for unstable/metastable phases). For such cases, the replacement of experimental data by ab initio calculations is desirable.

The accuracy of density-functional based ab initio methods is, in principle, only limited by the exchange-correlation (XC) functional. We have therefore evaluated the accuracy of the most commonly used functionals (LDA, GGA) by calculating key thermodynamic properties for a large set of metals (Al, Pb, Cu, Ag, Au, Pd, Pt, Rh, Ir). Great care was taken to ensure that convergence errors due to supercell size, k-point sampling, and energy cutoff are small compared to the error in the XC-functional. Based on the volume and temperature dependence of free energies calculated in the quasiharmonic approximation, thermodynamic quantities such as the thermal expansion or the heat capacity have been derived. The comparison to experiment yields an excellent agreement. A detailed analysis shows that the LDA/GGA results can typically be considered as error bars allowing to estimate the accuracy of the calculation in the absence of experiments.

MM 41.3 Fri 11:30 H16

Thermodynamische Berechnung von Pt-Basis-Legierungen — •Johannes Preussner, Rainer Völkl und Uwe Glatzel — Metallische Werkstoffe, Universität Bayreuth, Ludwig-Thoma-Str. 36b, 95447 Bayreuth

Platinbasislegierungen besitzen einen hohen Widerstand gegen korrosive Medien und gute mechanische Eigenschaften bei hohen Temperaturen. Durch eine geeignete Wahl an Legierungselementen und Wärmebehandlungsparametern kann eine den Nickelbasissuperlegierungen ähnliche Mikrostruktur eingestellt werden: in einer duktilen, Pt-reichen fcc-Matrix lassen sich feine $L1_2$ geordnete Pt_3Al Phasen ausscheiden. Das Legierungssystem Pt-Al-Cr-Ni hat sich dabei als sehr aussichtsreich erwiesen. Die Legierungsentwicklung wird durch thermodynamische Simulation unterstützt, um Vorhersagen über die Phasenbildung treffen zu können. Mit Hilfe von gezielten Experimenten (EDS, XRD) kann die Ausdehnung von Phasenregionen bestimmt werden. Ab-Initio Berechnungen geben hilfreiche Informationen über die Bildungsenthalpien einzelner Phasen. Diese Daten werden zusammen mit Literaturwerten dazu verwendet um die Gibbs-Energien $G(x,T)$ der einzelnen Phasen in Abhängigkeit von der Konzentration der Legierungselemente und der Temperatur zu bestimmen. Besonderes Augenmerk wird dabei auf die Pt-reiche Seite gelegt, da hier die Ordnungsreaktionen zu $L1_2$ stattfinden. Im Rahmen des Vortrags wird insbesondere die Thermodynamik des Systems Cr-Ni-Pt dargelegt.

MM 41.4 Fri 11:45 H16

Theory-guided design of Ti-based binaries for human implants — •Martin Friák[1], Jörg Neugebauer[1], Benedikt Sander[2], and Dierk Raabe[2] — [1]Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany — [2]Department of Microstructure Physics and Metal Forming, Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The improvement of hip transplants is severely hampered by the lack of suitable materials which are biocompatible in terms of non-toxicity and mechanical properties matched to the bone. The aim of our research has been therefore to identify metallurgical trends for non-poisonous Ti-based alloys employing quantum-mechanical calculations. Specifically, density functional theory (DFT), a plane wave basis set and PAW pseudopotentials have been used. As a first step the thermodynamic stability of Ti-Mo and Ti-Nb binaries has been determined. Second, the Young modulus of the thermodynamically stable alloys has been calculated and an alloy composition that maximally matches human bone has been selected. Guided by the theoretical calculations of phase stability and elastic properties, selected binaries were actually melted, cast, and heat treated to a homogeneous state. The samples have been experimentally characterized by x-ray methods, electron microscopy including crystallographic and chemical analysis, and mechanically tested using ultrasound measurements. The experimental data obtained in these experiments are in excellent agreement with the theoretical predictions.

MM 42: Materials design II

Time: Friday 12:30–13:30 Location: H16

MM 42.1 Fri 12:30 H16

A coupled meso-macro-scale simulation of solidification in Al-Cu alloys — •Ivaldo Leao Ferreira[1], Britta Nestler[1], and Amauri Garcia[2] — [1]Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany — [2]Fac. Engenharia Mecanica, UNICAMP, Brasil

The macroscopic heat transfer modelling associated to fluid flow is frequently used in prediction of ingots defects, while mesoscopic modelling is applied for the studies of alloy changes in relation to a typical microstructure. By combining a meso-scale model for the extraction of local alloy concentrations and a macro-scale model able to predict temperature, solute concentration, velocity fields and pressure profiles, it is possible to conduct cast process simulations for a large range of space and time scales. An extension of a 2D macro-scale model proposed for predicting inverse macrosegregation profiles during solidified alloy ingots is coupled with a meso-scale phase-field model for simulating microstructure formation processes. The phase-field model can provide parameters such as the phase fractions, primary/secondary arm spacings and microsegregation profiles. The approach will help to understand the effects exerted by the kinetics of solidification on the form of microstructure and consequently on microsegregation and macrosegregation profile in ingots or casting parts in commercially available alloys.

MM 42.2 Fri 12:45 H16

Parallel algorithms for microstructure simulations with fluid flow — •Michael Selzer and Britta Nestler — Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Fluid flow has an important effect on the formation of microstructures and on the properties of materials. Our numerical method for solving the Navier-Stokes equations coupled with the microstructure model is based on a finite difference method on a staggered grid including a successive overrelaxation iteration for the pressure update. Simulations modelling the ripening process of a fine distribution of liquid droplets embedded in a fluid medium have demonstrated the necessity of developing parallel and optimized algorithms for solving the set of nonlinear partial differential equations in order to reduce computing times. The parallelization is realized by a domain decomposition using the message passing interface (MPI) library for data exchanging between computing nodes. To homogenize the load distribution, a dynamic redistribution of the domain decomposition is implemented. We apply the parallel simulator to microstructure formation processes with fluid flow and systematically analyze the computational performance depending on the configuration setup and on the optimization methods.

MM 42.3 Fri 13:00 H16

Thermoelectric currents in weld pools — •Adrian Lange and Eckhard Beyer — Fraunhofer Institut für Werkstoff- und Strahltechnologie, Winterbergstraße 28, D-01277 Dresden

In order to achieve higher welding speeds and a better quality of the weld seam, external static magnetic fields are tested for laser beam welding. Experiments with fine grained steels and aluminium alloys show a reduction of the so called humping effect, an improvement of the top seam quality, and an influence on the cross section of the seam [1,2]. These phenomena depend on the orientation of the magnetic field. To explain that dependence, the existence of thermoelectrical currents was proposed in [1,2]. The interaction of that proposed currents with the external field shall generate a Lorentz force distribution in the weld pool which may be the reason for the observed phenomena.

Based on the Onsager relation for the thermoelectrical current density and the appropriate boundary conditions for the laser beam welding, thermoelectrical currents can be determined analytically [3]. Results for iron and aluminium are presented in a approximative two-dimensional geometry. Since measurements for the values of the thermoelectrical (Seebeck) coefficient of both materials are spare, different hypothetical material sets are tested and discussed.

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[3] J. Paulini, G. Simon, and I. Decker, J. Phys. D **23**, 486 (1990).

MM 42.4 Fri 13:15 H16

XANES-Messungen zur atomaren Umgebung von Mg in AlMgSiCu-Legierungen — •Torsten Staab[1], Karl Maier[1], Hartwig Modrow[2] und Esther Dudzik[3] — [1]Universität Bonn, Helmholtz Institut für Strahlen- und Kernphysik, Nussallee 14-16, 53115 Bonn — [2]Universität Bonn, Physikalisches Institut, Nussallee 12, D-53115 Bonn — [3]Hahn-Meitner Institut Berlin/Bessy, Albert-Einstein-Str. 15, 12489 Berlin

Größe und Verteilung nanoskaliger Cluster — sogenannter Guinier-Preston-Zonen — bestimmen die Festigkeit von Aluminiumlegierungen. Diese Cluster behindern die Bewegung von Versetzungen. Schweißbare Al-Legierungen für den Flugzeugbau (Airbus A380) enthalten neben Mg und Si als Hauptlegierungsbestandteile auch Kupfer. Nachdem XANES-Messungen an der Cu k-Kante Hinweise auf die atomare Umgebung von Kupfer liefern konnten, zeigen neuere XANES/NEXAFS-Messungen an der Mg k-Kante auch die atomare Umgebung dieses Legierungselementes durch den Vergleich von ab-initio Rechnungen mit experimentellen Daten. Während des Alterungsprozesses der Legierung ändert sich die chemische Zusammensetzung der Ausscheidungen und damit die lokale atomare Umgebung der Legierungselemente Kupfer und Magnesium.

MM 43: Mechanical properties II

Time: Friday 11:00–12:00 Location: H6

MM 43.1 Fri 11:00 H6

high strength nanoporous platinum prepared by dealloying — •haijun jin[1], dominik kramer[1], julia ivanisenko[1], and jörg weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Technische Physik, Universität des Saarlandes, Saarbrücken, Germany

Nanoporous metals prepared by dealloying, which have been proposed for technological applications due to its novel properties, are typically brittle even when the metal skeleton consists only of a ductile element like gold. Here, we report on the fabrication of a material which combines nanoporosity and large surface area with improved mechanical properties. A dual-phase Pt-Ag alloy, of which one phase is the silver-rich matrix and another the platinum-rich dendrites, was subjected to dealloying. The silver-rich matrix was dealloyed to form a nanoporous Pt structure. And the platinum-rich dendrites were stable and remained undissolved after dealloying, which are expected to act stabilizing against shear localization and critical crack propagation in nanoporous metals. Compared with Pt samples with uniform nanoporous structure, this composite-like material exhibits a high strength over 200 MPa and large plastic deformation prior to failure under compression.

MM 43.2 Fri 11:15 H6

Novel high-strength Fe-based composite materials with large plasticity — •Katarzna Werniewicz[1,2], Uta Kühn[1], Norbert Mattern[1], Jürgen Eckert[1], Uwe Siegel[1], Birgit Bartusch[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, ul. Woloska 141, 02-507 Warsaw, Poland

Among glass-forming alloy systems reported so far, Fe-based bulk metallic glasses play a special role. Compared to other amorphous al-

loys e.g. Zr-, Ti-based, such glasses show superior mechanical strength. However, due to the general brittleness their wider application as structural materials is strongly restricted. The alternative approach to overcome this defect is to design BMG composites. In this work we present a series of new Fe-Cr-Mo-Ga-(Si,C) composite materials derived from an Fe-Cr-Mo-Ga-C-P-B glassy alloy, with the aim to improve the ductility of this high-strength material. The effect of the composition and the phase formation on the resulting mechanical properties was investigated. It has been found that the formation of a complex microstructure, which essentially consists of soft Ga-rich dendrites embedded in a hard Cr- and Mo-rich matrix, leads to a material with excellent compressive mechanical properties. While the obtained values of true strength are comparable with data reported for Fe-Cr-Mo-Ga-C-P-B BMG, the values of true strain are greatly improved for investigated composites.

MM 43.3 Fri 11:30 H6

Texture and mechanical anisotropy of ultrafine-grained Al alloy AA6016 produced by accumulative roll bonding — •Werner Skrotzki[1], Ingwar Hünsche[1], Juliane Hüttenrauch[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 alloy AA6016 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 calculated the mechanical anisotropy of the advanced metal sheets will be discussed.

MM 43.4 Fri 11:45 H6

Cu-Ag-alloys: materials with combined optimum properties — •Julia Lyubimova[1], Jens Freudenberger[2], Alexandre Gaganov[3], and Ludwig Schultz[4] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [4]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

In the present work two alloys, namely Cu - 7wt.% Ag and Cu - 24wt.% Ag, were investigated. The combination of optimum mechanical and electrical properties of these alloys was achieved. The conductor shows a ultimate tensile strength of 1,2 GPa, a strain to failure of 1,6 % and an electrical conductivity of 60 % IACS. The mechanical properties can be improved e.g. by the deformation at low temperatures or by the addition of a third element. The effect of the deformation temperature and also the Zr - addition on the properties of these alloys will be discussed. In addition, the fatigue behaviour of cold worked Cu - Ag - alloys will be shown.

MM 44: Mechanical properties III

Time: Friday 12:30–13:30 Location: H6

MM 44.1 Fri 12:30 H6

Improved plasticity in structurally inhomogeneous bulk metallic glasses — •J. Das[1], S. Pauly[1], K. B. Kim[2], S. Yi[3], W. H. Wang[4], and J. Eckert[1] — [1]IFW Dresden,Institut für Komplexe Materialien, Postfach 27 01 16, D-01171 Dresden, Germany — [2]Department of Advanced Materials Engineering, Sejong University, 98 Gunja-dong, Gwangjin-gu, Seoul 143-747, Korea — [3]Department of Materials Science and Metallurgy, Kyungpook National University, Daegu, 702-701, Korea — [4]Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China

To circumvent the limited ductility of bulk metallic glasses (BMGs), heterogeneous materials with glassy matrix and different type and length-scale of heterogeneities (micrometer-sized second phase particles or fibers, nanocrystals in a glassy matrix, phase separated regions, variations in short-range order by clustering) have been developed in order to control the mechanical properties. As example, recent results obtained for Cu- and Ti-base structurally inhomogeneous bulk metallic glasses will be presented. This type of clustered glasses is able to achieve high strength together with pronounced work hardening and large ductility by controlling the instabilities otherwise responsible for early failure. We emphasize the possibilities to manipulate such spatially inhomogeneous glassy structures based on martensitic alloys in favor of either strength and ductility, or a combination of both and also discuss the acquired ability to synthesize such "M-glasses" in bulk form through inexpensive processing routes.

MM 44.2 Fri 12:45 H6

Deformation kinetics in Zr-based 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

While deformation and flow in crystalline materials can be generally described in terms of the underlying dislocation dynamics, a corresponding formalism for disordered systems is intrinsically less defined. The latter class of materials also includes amorphous metals, which, compared to their crystalline counterparts, exhibit higher yield strength and elastic strain limit, but unfortunately suffer from low ductility at room temperature due to the formation of highly-localized shear bands.

Detailed micromechanical analysis of Zr-based bulk metallic glasses at various temperatures and strain rates facilitate accurate measurements of the inhomogeneous flow kinetics. Our results suggest a micromechanical deformation mechanism based on two processes: shear displacement through the formation and propagation of shear transformation zones, and diffusive structural relaxation processes in the distorted structure. The latter cease below a critical temperature (or above a critical strain rate), resulting in the disappearance of flow instabilities (i.e. serrations) correlated with a change in the strain rate sensitivity. Based on these findings, a constitutive deformation model is presented and similarities with the dynamic strain aging effect known for crystalline metals are elucidated.

MM 44.3 Fri 13:00 H6

Mechanical properties of multicomponent Fe-based glassy alloys — •Uwe Siegel, Uta Kühn, and Jürgen Eckert — Leibniz Institute for Solid State and Materials Research Dresden, PF 27 01 16, D-01171 Dresden

We report on phase formation and mechanical properties of a multicomponent (Fe44,3Cr5Co5Mo12,8Mn11,2C15,8B5,9)98,5Y1,5 glass-forming alloy. The material was prepared as thin ribbons and in form of rods. The samples were investigated by X-ray diffraction, scanning and transmission electron microscopy and DSC measurements. The alloy shows a high glass forming ability (critical casting thickness 12 mm) and high compressive strength (˜3000 MPa) but no yielding and strain hardening during room temperature deformation [1]. Therefore the alloy was used as a starting material for investigations concerning the improvement of the mechanical properties. The influence of heat treatments and composition changes on the phase formation and mechanical properties were examined. The strength of (Fe44,3Cr5Co5Mo12,8Mn11,2C15,8B5,9)98,5Y1,5-alloy was found to increase up to ˜3500 MPa by the replacement of Cr by Co and up to ˜4000 MPa by the replacement of Co by Cr. The addition of elements like Nb or Ag leads to a two phase microstructure consisting of an amorphous matrix and crystalline phases. The microstructure and the mechanical properties of these alloys will be presented.

References: [1] Z. P. Lu, C. T. Liu, J. R. Thompson, W. D. Porter, Phys. Rev. Lett. 92 (2004) 24.

MM 44.4 Fri 13:15 H6

compatible composition profiles and critical sizes of alloyed quantum dots — •huiling duan — Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76133 Karlsruhe, Germany

The assessment of composition profiles and strains is important to both the identification of the dominant growth mechanisms and the mod-

eling of the confining potential of alloyed quantum dots (QDs). We present first a compatibility equation for the misfit strains in alloyed QDs induced by the mismatch in the lattice constants or the thermal expansion coefficients of their alloying elements and show that it imposes some important restrictions on the alloy composition profiles. We then solve the strain field in embedded alloyed QDs induced by the nonuniform misfit strains. It is found that the induced field is uniform if the misfit strains satisfy the compatibility equation, but not otherwise. Finally, we consider the energy of nucleation of a circular prismatic dislocation loop to relieve the misfit strain and calculate the critical size of a dislocation-free alloyed QD. We show that this size is much larger when the alloy composition meets the restrictions imposed by the strain compatibility equation than when it does not.