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

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Overview of Invited Talks and Sessions

(lecture IFW A, IFW B, and IFW D; Poster P4)

Invited Talks

MM 1.1	Mon	10:15–10:45	IFW A	**Fabrication and Properties of Nanoporous Metals by Electrochemical Dealloying** — •Jonah Erlebacher
MM 7.1	Mon	14:00–14:30	IFW A	**Non-destructive residual stress analysis with neutrons** — •Michael Hofmann
MM 12.1	Tue	9:30–10:00	IFW A	**Small scale mechanical testing: Challenges and benefits** — •Gerhard Dehm
MM 13.1	Tue	10:15–10:45	IFW A	**Small-Angle Neutron Scattering in Materials Science** — •Pavel Strunz, Debashis Mukherji, Gerhard Schumacher, Ralph Gilles, Albrecht Wiedenmann
MM 14.1	Tue	11:45–12:15	IFW A	**Anomalous small-angle X-ray scattering in material science** — •Armin Hoell
MM 19.1	Tue	14:00–14:30	IFW A	**Diffusion, interface shifts and solid state reactions in nanoscale** — •Dezso L. Beke, Zoltan Erdélyi, Zoltan Balogh, Csaba Cserháti, Gabor A. Langer, Gabor L. Katona
MM 24.1	Wed	9:30–10:00	IFW A	**From eutectic alloys to metal nanowires** — •Achim Walter Hassel
MM 30.1	Wed	14:00–14:30	IFW A	**Precipitation-hardening of aluminium alloys - challenges and recent developments** — •John Banhart
MM 36.1	Thu	9:30–10:00	IFW A	**Onset of plasticity as observed by force microscopy** — •Roland Bennewitz

Joined Symposium Chemical Reactions on Nanomaterials: Progress from in-situ Experimental Studies and Theoretical Investigations (SYCR)

Together with CPP, O, DS and VA

In application fields ranging from fuel cells and chemical production to electronic sensors for automotive and environmental monitoring the dream of a rational design of improved catalysts is still elusive. Making this dream a reality ultimately requires an atomic-scale understanding of the complex surface reaction behaviour under realistic operation conditions of the employed multi-component materials, typically composed of metal or alloy nanoparticles supported on an oxide substrate. This involves microscopic details such as the adsorption on different nanoparticle facets, dissolution of gas atoms in the bulk of the nanoparticles, and adhesion to the oxide substrate and thus unites aspects from surface science, material science, as well as physical chemistry.
Substantial effort has been devoted within the past few years to develop new experimental and theoretical techniques capable of delivering such atomic-scale information on surfaces and nanoparticles under reaction conditions, thereby bridging the "pressure gap"from ultra-high vacuum to atmospheric pressures and the materials gap from single crystal (metal) surfaces to (supported) nanoparticles. This symposium will highlight corresponding studies, focusing in particular on the evolution of the active material in technologically relevant environments as e.g. illustrated by the controversially discussed formation of sub-nanometer thin surface oxide layers in oxidation catalytic applications.
Organizers:

Dr. Andreas Stierle
Max Planck Institut für Metallforschung, Heisenbergstraße 3 D-70569 Stuttgart
Prof. Dr. Reinhard Denecke
Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Physikalische Chemie II, Universität Leipzig, Linnéstraße 2, D-04103 Leipzig
PD Dr. Karsten Reuter
Fritz-Haber-Institut, Abt. Theorie, Faradayweg 4-6, D-14195 Berlin

Invited talks of the joint symposium SYCR

See SYCR for the full program of the Symposium.

SYCR 1.1	Thu	14:00–14:30	BAR SCHÖ	**Reactivity trends in CO oxidation from ultrahigh vacuum to elevated pressures** — •Wayne Goodman
SYCR 1.2	Thu	14:30–15:00	BAR SCHÖ	**Ruthenium oxide as oxidation catalyst** — •Robert Schlögl, Dirk Rosenthal, Frank Girsdies, Raoul Blume, Olaf Timpe
SYCR 1.3	Thu	15:00–15:30	BAR SCHÖ	**Low dimensional surface oxides in the oxidation of Rh particles** — •Florian Mittendorfer
SYCR 1.4	Thu	16:00–16:30	BAR SCHÖ	**In-situ microscopy of chemical reactions on transition metal surfaces** — •Peter Sutter
SYCR 1.5	Thu	16:30–17:00	BAR SCHÖ	**Live STM and X-ray observations of catalytic processes** — •Joost W.M. Frenken
SYCR 1.6	Thu	17:00–17:30	BAR SCHÖ	**Computational materials design: Alloys for selective hydrogenation catalysis** — •Thomas Bligaard

Topical Sessions

Topical Session Nanoporous Functional Materials
Porous materials combine aspects of granular matter, in particular the large number of surfaces, with behaviour that is characteristic of solids, such as mechanical strength. This has brought porous solids into focus for use as functional materials. Some substances order spontaneously into crystalline structures with regular arrays of interstices, for example, zheolites. Yet, even metals or semiconductors which, conventionally, tend to form bulk materials owing to the trend of nature to spontaneously minimize the area of surface, can be made porous by proper synthesis. This includes in particular the controlled chemical or electrochemical corrosion of elemental semiconductors or of metal alloys. Nanoporous solids represent the lower end of the size scale that can be reached in this way, and the upper end of surface-to-volume ratio. Recent research on nanoporous materials has brought up intriguing science under a variety of aspects, reaching from quantum confinement over sensors and catalysis up to electrochemical tuning of materials properties and size effects in plasticity. In addition, nanoporous materials may serve as template for nanostructuring.
The symposium intends to provide a forum for scientific exchange in this interdisciplinary field of nanoporous functional materials.
Organizers:
Univ.-Prof. Dr. Roland Würschum
Technische Universität Graz, Institut für Materialphysik, Petersgasse 16, A-8010 Graz
PD Dr. Jörg Weissmüller
Institut für Nanotechnologie, Forschungszentrum Karlsruhe GmbH, PO-Box 3640, D-76247 Karlsruhe

Topical Session Nanoanalytics using Small-Angle Scattering with X-rays, Neutrons and Electrons
Small-angle scattering with X-rays, neutrons and even with electrons provides information about features in heterogeneous materials that have sizes on the length scale from typically 2 to 200 nm. Unlike the usual wide-angle Bragg scattering one can therefore characterise the mesostructure of a variety of materials ranging from metals, ceramics, polymers, glasses to complex liquid matter. Chemical sensitivity is provided either by energy variation (X-rays) or isotopic substitution (neutrons). In the latter case, polarisation can also provide magnetic contrast.
The challenges associated with these techniques are manifold: the small-angle scattering signal has to be measured very precisely and the mathematics of evaluating data and deriving a physical model

is challenging. Real-time and in-situ techniques are becoming more popular and require additional efforts.
In this symposium we want to review the recent developments of measurement techniques, the mathematical algorithms and models and present current application examples.
Organizer:
Prof. Dr. John Banhart
Helmholtz Centre Berlin for Materials and Energie, Department of Materials (SF3), Glienicker Str. 100, D-14109 Berlin

Topical Session High Temperature Materials
Fundamental research in high temperature materials is necessary to achieve higher efficiency in transportation and power generation systems. The improvement of established structural materials as nickel-base superalloys is necessary but also the development of new structural material classes as high temperature intermetallics, refractory alloys and coatings. For this an in-depth understanding of the physical processes occurring in the base material and coatings is necessary. Research topics in these often complex multi-component materials are phase transformations and phase constitution either under equilibrium or non-equilibrum conditions, the fundamentals of deformation mechanisms on the nanometer and atomic scale and diffusion controlled processes connected with precipitation, corrosion and a large number of other phenomena. Here the employment of advanced characterization methods like transmission electron microscopy and different diffraction techniques in combination with measurements of the local and global mechanical properties is necessary. These experimental work needs to be connected with modeling on different length scales to fully comprehend the complicated mechanisms occurring in high temperature materials.
The symposium will present the recent progress in several invited talks by leading experts in this field.
Organizers:
Prof. Dr. Mathias Göken
Institut für Werkstoffwissenschaften I, Universität Erlangen-Nürnberg, Martensstrasse 5, D-91058 Erlangen
Dr. Florian Pyczak
GKSS-Forschungszentrum Geesthacht GmbH, Abteilung Metallphysik, Max-Planck-Strasse 1, D-21502 Geesthacht
Prof. Dr. Martin Heilmaier
Otto-von-Guericke-Universität Magdeburg, Institut für Werkstoff- und Fügetechnik, Universitätsplatz 2, D-39106 Magdeburg

Sessions

MM 1.1–1.4	Mon	10:15–11:45	IFW A	**Topical Session Nanoporous Functional Materials I**
MM 2.1–2.3	Mon	12:00–13:00	IFW A	**Topical Session Nanoporous Functional Materials II**
MM 3.1–3.4	Mon	10:30–11:30	IFW B	**Mechanical Properties I**
MM 4.1–4.5	Mon	11:45–13:00	IFW B	**Mechanical Properties II**
MM 5.1–5.6	Mon	10:15–11:45	IFW D	**Materials Design I**
MM 6.1–6.4	Mon	12:00–13:00	IFW D	**Materials Design II**
MM 7.1–7.1	Mon	14:00–14:30	IFW A	**HV Hofmann**
MM 8.1–8.4	Mon	14:45–16:30	IFW A	**Topical Session Nanoporous Functional Materials III**
MM 9.1–9.4	Mon	14:45–15:45	IFW B	**Intermetallic Phases I**
MM 10.1–10.3	Mon	16:00–16:45	IFW B	**Intermetallic Phases II**
MM 11.1–11.6	Mon	14:45–16:15	IFW D	**Growth**
MM 12.1–12.1	Tue	9:30–10:00	IFW A	**HV Dehm**
MM 13.1–13.4	Tue	10:15–11:30	IFW A	**Topical Session Nanoanalytics using Small-Angle Scattering I**
MM 14.1–14.3	Tue	11:45–12:45	IFW A	**Topical Session Nanoanalytics using Small-Angle Scattering II**
MM 15.1–15.3	Tue	10:15–11:15	IFW B	**Topical Session Nanoporous Functional Materials IV**
MM 16.1–16.4	Tue	11:30–12:30	IFW B	**Diffusion and Point Defects I**
MM 17.1–17.6	Tue	10:15–11:45	IFW D	**Mechanical Properties III**
MM 18.1–18.4	Tue	12:00–13:00	IFW D	**Mechanical Properties IV**
MM 19.1–19.1	Tue	14:00–14:30	IFW A	**HV Beke**
MM 20.1–20.21	Tue	14:45–16:30	P4	**Poster Session I**
MM 21.1–21.9	Tue	14:45–16:30	P4	**Topical Session Nanoporous Functional Materials - Poster**

MM 22.1–22.2	Tue	14:45–16:30	P4	**Topical Session Nanoanalytics using Small-Angle Scattering - Poster**
MM 23.1–23.11	Tue	14:45–16:30	P4	**Topical Session Heterogeneous Nucleation and Initial Evolution of Microstructure - Poster**
MM 24.1–24.1	Wed	9:30–10:00	IFW A	**HV Hassel**
MM 25.1–25.6	Wed	10:15–12:15	IFW A	**Topical Session High Temperature Materials I**
MM 26.1–26.4	Wed	10:15–11:15	IFW B	**Nanostructured Materials I**
MM 27.1–27.5	Wed	11:30–12:45	IFW B	**Interfaces I**
MM 28.1–28.6	Wed	10:15–11:45	IFW D	**Electronic Properties I**
MM 29.1–29.4	Wed	12:00–13:00	IFW D	**Diffusion and Point Defects II**
MM 30.1–30.1	Wed	14:00–14:30	IFW A	**HV Banhart**
MM 31.1–31.5	Wed	14:45–16:30	IFW A	**Topical Session High Temperature Materials II**
MM 32.1–32.4	Wed	16:45–18:00	IFW A	**Topical Session High Temperature Materials III**
MM 33.1–33.7	Wed	14:45–16:30	IFW B	**Phase Transitions I**
MM 34.1–34.7	Wed	14:45–16:30	IFW D	**Liquid and Amorphous Metals I**
MM 35.1–35.42	Wed	16:30–18:30	P4	**Poster Session II**
MM 36.1–36.1	Thu	9:30–10:00	IFW A	**HV Bennewitz**
MM 37.1–37.6	Thu	10:15–12:00	IFW A	**Topical Session High Temperature Materials IV**
MM 38.1–38.6	Thu	10:15–11:45	IFW B	**Nanostructured Materials II**
MM 39.1–39.4	Thu	12:00–13:00	IFW B	**Phase Transitions II**
MM 40.1–40.5	Thu	10:15–11:30	IFW D	**Quasicrystals I**
MM 41.1–41.5	Thu	11:45–13:00	IFW D	**Interfaces II**
MM 42.1–42.7	Thu	14:00–15:45	IFW A	**Nanostructured Materials III**
MM 43.1–43.7	Thu	16:00–17:45	IFW A	**Liquid and Amorphous Metals II**
MM 44.1–44.4	Thu	14:00–15:00	IFW B	**Quasicrystals II**
MM 45.1–45.5	Thu	15:15–16:30	IFW B	**Phase Transitions III**
MM 46.1–46.5	Thu	16:45–18:00	IFW B	**Electronic Properties II**
MM 47.1–47.7	Fri	10:15–12:00	IFW A	**Liquid and Amorphous Metals III**
MM 48.1–48.7	Fri	10:15–12:00	IFW B	**Nanostructured Materials IV**
MM 49.1–49.6	Fri	10:15–11:45	IFW D	**Hydrogen in Metals**

Annual General Meeting Metal and Material Physics Division

Wednesday 18:30–19:30 Room IFW B

- Report of the chairman of the Metal and Material Physics Division.
- Invited talks and symposia for the next spring meeting 2010.
- Other topics.

MM 1: Topical Session Nanoporous Functional Materials I

Time: Monday 10:15–11:45 Location: IFW A

Invited Talk MM 1.1 Mon 10:15 IFW A

Fabrication and Properties of Nanoporous Metals by Electrochemical Dealloying — •Jonah Erlebacher — Johns Hopkins University, Baltimore, MD

Dealloying, the electrochemical selective dissolution of a multicomponent alloy, is an intrinsically nanoscale phenomena that under the right conditions leads to the formation of highly porous metals due to an atomic-scale competition between electrochemical dissolution and crystalline surface diffusion of the remaining components. Recent attention in this area is focused toward practical application of dealloying to form "nanoporous" metals with pore sizes less than 10 nm possessing ultra-high surface areas. Nanoporous metals formed by dealloying are microstructurally contiguous porous single crystal networks, and not fragile sintered agglomerations of nanoparticles. For this reason, they are finding many new applications in sensing and catalysis.

In this presentation, we will describe the evolution of the beautiful nanoporous microstructure of dealloyed metals and their applications in a variety of contexts. We will also discuss the use of a minority ternary component in the alloy precursors that stymie surface mobility along step edges, stabilizing the nanoporous morphology during dealloying, and the use of electrochemical tricks to control the surface composition of the nanoporous metal. Finally, we will discuss the development of new nanoporous metals that exhibit remarkable catalytic activity, particularly toward chemical reactions important to energy technologies, such as oxygen reduction in fuel cells

Topical Talk MM 1.2 Mon 10:45 IFW A

The role of surface chemistry on the properties of nanoporous gold — •Juergen Biener[1], Arne Wittstock[1,2], Luis A. Zepeda-Ruiz[1], Monika M. Biener[1], Volker Zielasek[2], Dominik Kramer[3], Raghavan N. Viswanath[3], Joerg Weissmüller[3], Marcus Baeumer[2], and Alex V. Hamza[1] — [1]Nanoscale Synthesis and Characterization Laboratory, Lawrence Livermore National Laboratory, USA — [2]Institut für Angewandte und Physikalische Chemie, Universität Bremen, Germany — [3]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany

Although surfaces or, more precisely, surface atoms determine the way how materials interact with their environment, the influence of surface chemistry on the bulk of the material is generally considered to be small. However, in the case of high surface area materials such as nanoporous gold the influence of surface properties can no longer be neglected. Therefore, actively controlling surface properties such as diffusion barriers and surface stress by surface chemistry should provide an opportunity to manipulate and fine-tune material properties. Specifically, we will show that surface chemistry is an important factor in determining the stability of nanostructured gold surfaces, and that macroscopic strain can be generated by surface-chemistry induced changes of the surface stress. The latter effect can be used to directly convert chemical energy into a mechanical response without generating heat or electricity first and thus opens the door to surface-chemistry driven actuator and sensor technologies. Prepared by LLNL under Contract DE-AC52-07NA27344.

MM 1.3 Mon 11:15 IFW A

Electrochemical actuation using nanoporous metals — •Viswanath Raghavan Nadar[1], Dominik Kramer[1], and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Technische Physik, Universität des Saarlandes, Saarbrücken, Germany

Actuating in response to an electric stimulus is well known for solid insulators, for instance piezo-ferroelectrics and conducting polymers, where an electric field penetrating the sample creates bulk distortion. The more recent observation of reversible dimension changes in nanoporous metal electrodes exploits different physics: Varying the electrode potential results in the formation of double layer, with a local electric field that is screened in the surface region. Changes in the mean surface atom bonding, due to the excess charge, modify the capillary forces at the surface, and bulk strain is required to set up a compensating stress throughout the lattice. Owing to their large specific surface area and large capacity, nanoporous Pt, Au, Pd wetted by electrolytes will thus exhibit reversible volume changes when their potential is varied. In a suitable setup, the action can be seen with the naked eye. In-situ dilatometry studies on these metals demonstrate that the variation of reversible strain is a linear function with charge. This highlights the distinction of the underlying capillary parameter, the surface stress, from the surface tension. Outside of the double layer regime, the stress-charge response reflects, among other factors. Thus, experiments on actuation of nanoporous metals provide insights into the microscopic processes at the electrochemical interface.

MM 1.4 Mon 11:30 IFW A

A light-weight, large strain nanoporous actuator material that can be used in compression — •Lihua Shao[1], Jürgen Biener[2], Dominik Kramer[1], Viswanath Raghavan Nadar[1], Theodore F. Baumann[2], and Jörg Weissmüller[1] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Lawrence Livermore National Laboratory, Livermore, California, USA

Considerable progress has been made about the charge induced strain of nanoporous materials. Possible actuator applications have been suggested for noble metals and carbon nanotubes. The high costs of such materials are an impediment to application, as the fact that carbon nanotube arrays cannot be loaded in compression. It is therefore of interest to search for alternative materials which combine mechanical and chemical stability with low cost. We will report first results on the mechanical and electrochemical properties of a light-weight, bulk material with extremely large surface area that can be used in compression, and that achieves a reversible strain of 0.45%. Besides actuation applications, nanoporous solids impregnated by electrolyte are also of interest with regards to the measurement of a fundamental parameter, namely the potential of zero charge (pzc). For liquid metals the pzc coincides with the maximum of the surface tension, from which it can be measured. However, the strain of solids is governed by the surface stress, which is not a maximum at the pzc. We measured the pzc and the charge-dependent strain in various electrolytes and excluded an agreement between pzc and the potential of length minimum.

MM 2: Topical Session Nanoporous Functional Materials II

Time: Monday 12:00–13:00 Location: IFW A

Topical Talk MM 2.1 Mon 12:00 IFW A

Plastic deformation of macroscopic nanoporous metals — •Hai-Jun Jin — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany

Mechanical behavior of nanoporous metals reflects the collective deformation of extended arrays of nano-objects. Studies of their intrinsic mechanical properties have been prevented by high density of preformed cracks and thereby the severe brittleness of bulk nanoporous samples. This presentation will focus first on the strategies to fabricate macroscopic crack-free and high strength nanoporous metals, and then the experimental studies on the mechanical performance of monolithic and crack-free nanoporous gold samples. Millimeter-sized nanoporous gold samples can be prepared with excellent ductility in compression, enabling studies of the yield phenomenon and strain rate sensitivity along with the microstructure evolution. A distinguishing collective feature of deformation will be discussed in this material, in relation to its long range coherent crystal lattice at a scale much larger than the ligament size. (The following collaborations are acknowledged: D. Kramer, L. Kurmanaeva, Y. Ivanisenko, J. Weissmüller, INT, FZ Karlsruhe; J. Schmauch, Uni. Saarlandes; H. Rösner, Uni. Münster; DFG Forschergruppe 714 'Plastictiy of Nanocrystalline Solids')

MM 2.2 Mon 12:30 IFW A

Elastic properties and freezing of argon confined in meso-

porous glass — •Klaus Schappert and Rolf Pelster — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus E 2.6, 66123 Saarbrücken, Germany

We study the properties of argon adsorbed in mesoporous Vycor glass with a mean pore diameter of 8 nm. Our ultrasonic measurements show, that below the freezing point of argon the adsorption process proceeds in three steps [1]. The first few adsorbed wall-layers remain liquidlike; i.e., freezing starts only at a temperature dependent filling of the pores. At a somewhat higher filling of the porous sample, we observe an abrupt increase of the effective shear modulus to a plateau value. From the dependence of the effective shear modulus on the filling fraction and the temperature, we infer some elastic properties of the adsorbed argon itself.

[1] Klaus Schappert and Rolf Pelster, Phys. Rev. B 78, 174108 (2008)

MM 2.3 Mon 12:45 IFW A

Nanoporous Superalloys by Selective Phase Extraction: Processing, Properties, Applications — •Joachim Rösler, Oliver Näth, and Fabian Schmitz — Technische Universität Braunschweig, Langer Kamp 8, D-38106 Braunschweig

Nanoporous Ni-based superalloys are a new material class [1]. They are fabricated from sheets of the two phase g/g* base material by thermomechanical processing, followed by selective phase extraction of either the g- or g*-phase. As a result, a porous membrane is obtained, containing extremely regular and fine channel-like porosity on the nanoscale. First, manufacturing of these materials is described and considerable flexibility in controlling the pore morphology is demonstrated. Furthermore, (micro-)structuring of the membranes in solid and porous domains as well as coating processes for external and internal material deposition are illustrated. These options are of particular interest, e.g. for the design of micro-chemical reactors, heat exchangers or Pd-based oxygen membranes. Secondly, microstructure-property correlations are discussed and it is demonstrated that the thermomechanical processing parameters critically control mechanical strength and gas permeability. Tensile strength levels of up to 100 MPa are achieved when the processing parameters are adjusted accordingly. At the same time, molecular separation of gas mixtures is possible as the pore dimensions are comparable to the mean free path of the gas molecules. This may be of particular interest for the separation of hydrogen.

[1] J. Rösler, O. Näth, S. Jäger, F. Schmitz and D. Mukherji, Acta Mater., 53, 1397 (2005)

MM 3: Mechanical Properties I

Time: Monday 10:30–11:30 Location: IFW B

MM 3.1 Mon 10:30 IFW B

Periodic Phase Composites in Aluminide Thin Films Produced by Laser Interference Metallurgy - Mechanical and Structural Characterisation — •Peter Leibenguth, Eric Detemple, and Frank Mücklich — Department of Materials Science and Engineering, Functional Materials, Saarland University, Saarbrücken, Germany

Laser Interference Metallurgy is a straightforward means of producing thin film composite materials. By overlapping two or more coherent laser beams on the material surface, an interference pattern can be achieved. Its periodic arrangement of intensity maxima and minima allows the formation of a controlled laterally patterned structure of processed and directly neighbouring unprocessed regions in micronscale. Besides melting, annealing and recrystallisation, the Laser processing can induce the formation of other phases having significantly different properties.

We concentrate on the effects of this treatment on the mechanical properties of multilayered thin films, whose composition allows the formation of mechanically interesting aluminide phases. For this purpose, we use a nanosecond-pulsed Nd:YAG laser with high peak power whose primary beam is split in two sub-beams by an appropriate beam-splitter and mirror setup. The resulting composite consists of a periodic array of hard and ductile phases. Structure determination is performed by GI-XRD and TEM. Using bulge-testing and nanoindentation, the global and local mechanical properties are analysed.

MM 3.2 Mon 10:45 IFW B

Experimental based calibration for strain measurement in silicon with Raman spectroscopy — Natallia Zhlobich, Martin Küttner, Henning Heuer, and •Jörg Opitz — Fraunhofer IZFP-D, Dresden, Germany

Raman Spectroscopy becomes more and more important in research and development i.e. for pharmaceutical, chemical or biological applications. Also in semiconductor or photovoltaic industries Raman spectroscopy on Silicon will be an important method to measure strain and chemical-physical interactions. To increase spatial resolution for near field Raman spectroscopy with a basically weak intensity an optimization problem between fast measurements versus perfect peak quality has to be solved. Different parameters of the experiment are used to improve the quality of Raman peaks and to decrease the exposure time. Applied stress in the samples is calculated with help of a theoretical model for 4 point bending. The dependance between mechanical stress and Raman shift is obtained. The influence of different parameters of the experiment on the interpretation of Raman data is discussed. The results of this work will be used in the further developing of a Scanning Near-field Optical Microscopy technique for stress mapping with high spatial resolution.

MM 3.3 Mon 11:00 IFW B

Anharmonic contributions to the phonon density of states of rock-salt AlN — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

The standard approach to calculate the phonon dispersion of crystals by means of density functional theory is based on the harmonic approximation. Unfortunately, this method is limited to 0 K calculations and neglects anharmonic contributions completely.

Molecular dynamics simulations allow to obtain the phonon density of states (PDOS) by Fourier transformation of the velocity autocorrelation function. This route opens the way to study phases at various temperatures and also includes anharmonic contributions to the PDOS.

We compare the results of both methods in case of several AlN phases, which are of recent experimental and theoretical interest. In particular we focus on the vibrational properties of the cubic AlN phase.

We would like to thank the DFG for financial support within the DFG Priority Program 1236: *Strukturen und Eigenschaften von Kristallen bei extrem hohen Drücken und Temperaturen*

MM 3.4 Mon 11:15 IFW B

Effect of residual stresses on fatigue crack propagation of friction stir welded joints — Torben Fischer[1], •Peter Staron[1], Jorge dos Santos[1], Yu-E Ma[2], and Andreas Schreyer[1] — [1]GKSS Research Centre, Max-Planck-Str. 1, 21502 Geesthacht, Germany — [2]Cranfield University, Cranfield Bedfordshire, MK43 0AL, United Kingdom

Friction stir welding (FSW) is a proven technology for use in airframes. FSW is now seen as a key element for producing cost effective integral metallic structures in future airframe applications. By further understanding and development of the FSW process new applications can be realized leading to further cost and weight benefits for metallic airframe structures, which will make these structures more competitive in the future. Of particular importance is the understanding of the effect of residual stress on the performance of the welded components. In order to investigate the influence of the sample dimensions on maximum residual stresses and fatigue crack growth, fatigue test samples with different sizes of a batch of friction stir welded AA 2195 sheets were tested. A crack-initiating notch was inserted perpendicular to the weld line on the advancing side of the weld. Residual stress measurements have been carried out with the neutron diffractometer ARES-2 at Geesthacht Neutron Facility (GeNF). First results show that the residual stresses depend strongly on the specimen size and that the fatigue crack propagation speed depends on the residual stress state.

MM 4: Mechanical Properties II

Time: Monday 11:45–13:00 Location: IFW B

MM 4.1 Mon 11:45 IFW B

Crystal plasticity finite element study on small scale plasticity of micropillars — •D. Ma[1], D. Raabe[1], F. Roters[1], R. Maass[2], and H. Van Swygenhoven[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany — [2]Paul Scherrer Institute, CH-5232 Villigen, Switzerland

Experimental studies on micro-compression testing on single crystals reveal that these samples are stronger than the respective bulk material. The onset of plasticity is hard to determine from the stress-strain curves, however, it can be associated with changes in in-situ taken Laue patterns. This method allows one to identify the true start of plastic yielding of such single crystals which is referred to as "Laue-yield". By applying this concept, recent experimental work discovered that the trend of smaller is stronger is considerably reduced (*Van Swygenhoven et al., in press*). In these experiments it has been observed that unexpected slip systems non-Schmid planes are activated prior to the geometrically predicted ones on Schmid planes. We use a crystal plasticity finite element method for investigating the details of the slip system activation under different boundary conditions, such as minor orientation and shape deviations of the crystals used, different contact conditions between sample and compression tools, and possible misalignments of the compression tools. In this study, we show how those boundary conditions influence the micro-compression test, the active slip system, and even the measured stresses. The results reveal that under certain small tool misalignments (ca. 2°) the activation of unexpected slip systems with small Schmid factors can be explained.

MM 4.2 Mon 12:00 IFW B

Evolution of Vickers hardness during room temperature grain growth of nanocrystalline Palladium — •Christian Braun[1], Jörg Schmauch[1], Jürgen Markmann[1,2], and Rainer Birringer[1] — [1]Universität des Saarlandes, FR 7.3 Technische Physik, Campus D2.2, 66123 Saarbrücken — [2]Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen

Indentation methods provide a fast and reliable mean to characterize plastic deformation and hardness. Based on hardness values the Tabor relation allows one also to estimate yield strength. For polycrystalline coarse grained materials the Hall-Petch equation describes the relation between materials strength and its grain size. There are many studies, theory and experiment, around that corroborate that in nanometer-sized polycrystalline materials Hall-Petch behaviour prevails. Uncovering the physics of plastic flow in bulk nanocrystalline materials requires detailed studies of the scaling behaviour of yield stress versus grain size. With the recent discovery of room temperature grain growth in nc Palladium, it becomes feasible to investigate the scaling behaviour starting out from grain sizes below 10 nm up to the micrometer scale. In this study, we report about the evolution of Vickers hardness and strain rate sensitivity of nc Palladium during room temperature grain growth.

MM 4.3 Mon 12:15 IFW B

***In-situ* SEM micropillar compression of Zr-based bulk metallic glasses with different free volume content** — •Alban Dubach[1,2], Johann Michler[2], Upadrasta Ramamurty[3], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, ETH Zurich, Wolfgang-Pauli-Str. 10, 8093 Zürich, Switzerland — [2]EMPA Materials Science and Technology, Feuerwerkerstrasse 39, 3602 Thun, Switzerland — [3]Department of Materials Engineering, Indian Institute of Science, Bangalore-560012, India

In contrast to crystalline metals, which exhibit dislocation-mediated deformation, bulk metallic glasses (BMGs) usually exhibit high yield strength and a plastic deformation which is triggered by free volume. Under an applied stress, clusters of atoms with high free volume (i.e. "shear transformation zones", STZs) accommodate shear strains locally. At room temperature these STZs coalesce along planes of maximum shear stress, leading to a deformation which is spatially and temporally restricted within narrow shear bands and therefore difficult to assess experimentally. In this study the uniaxial compression of micrometer-sized pillars has been investigated *in-situ* inside a scanning electron microscope. The micropillars, having diameters between 0.3 and 3 μm, were fabricated by focused-ion beam milling of a Zr-based BMG in three different conditions: as-cast, structurally-relaxed and shot-peened. Effects of different free volume content, sample size and applied strain rate have been analyzed. Shear band formation and stable propagation is observed to be the plastic deformation mode, with no difference in yield strength according to either size or condition.

MM 4.4 Mon 12:30 IFW B

Discrete dislocation dynamics study of the influence of boundary conditions in micro-samples — •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

Ongoing miniaturization in technical devices demands a better understanding of mechanical properties of metallic structures in micro-meter range. Compression and tension tests on single crystalline samples revealed a size-dependency of flow stress. With decreasing pillar diameter an increasing average flow stress and an increasing standard deviation. Experimental uncertainties in the control of the deformation, like misalignment between sample and loading device can occur, leading to more complex stress states than desired, e.g. superimposed torsion or bending moments. Three dimensional discrete dislocation dynamics simulations are performed to explore the effect of superimposed torsion moments on tensile experiments. Samples with variable diameters and aspect ratio are also loaded with uniaxial tensile stresses and different boundary conditions, different allowed displacements of the top surface of the micro pillars. Identical initial dislocation structure for different loading conditions shows clearly the impact of the boundary conditions on the observed plastic behavior and internal dislocation micro structure. Source activation and active glide planes are influenced by boundary conditions as torsion moments activate other sources than tensile stresses.

MM 4.5 Mon 12:45 IFW B

Research into the parallel determination of Young's modulus E and Poisson's ratio ν via normal and lateral nanoindentation experiments — •Andre Clausner and Frank Richter — TU-Chemnitz, Institut für Physik, Germany

In the case of a lot of materials used in various technical applications the assumption of isotropic behaviour can be made. For these materials the most important mechanical properties needed, for example for an FE-simulation of specific geometries, are the Young's modulus E and the Poisson's ratio ν. These material constants have to be determined experimentally on a existing structure which is most comparable with the later application. Therefore, as well as for small structures and thin film applications, a very small impact size and depth of the experiment on the structure is favoured. For this purposes instrumented nanoindentation experiments with different indenter shapes are used. In the case of the Young's modulus we can obtain the value of E via the well know Oliver and Pharr method for instrumented indentation experiments in normal direction. To obtain a second material constant, a second experiment is needed, independent from the normal one. A lateral displacement of a normal loaded spherical indenter in the range of sticking friction is used. For this mechanical loading situation there are some simplified analytical solutions in the elastic theory. Via comparison of the measured lateral data and the analytical model predictions the Poisson's ratio can be determined. The talk wants to show the possibilities and the recently obtained results of this proceeding to determine ν.

MM 5: Materials Design I

Time: Monday 10:15–11:45 Location: IFW D

MM 5.1 Mon 10:15 IFW D

Using ab initio calculations in designing bcc Mg-Li alloys for ultra light-weight applications — William Art Counts, •Martin Friák, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. In order to explore the suitability of this approach in identifying potential candidates for ultra-light-weight applications we studied bcc Mg-Li alloys. In a first step, the fundamental physical properties (like formation energy and elastic constants) of an extensive set of bcc Mg-Li compounds are calculated using density-functional theory (DFT) and compared with available experimental data. These DFT-determined properties are in turn used to calculate engineering parameters like (i) specific Young's modulus (Y/ρ) or (ii) bulk over shear modulus ratio (B/G) differentiating between brittle and ductile behavior. In a second step, these engineering parameters are used to identify alloys that have optimal mechanical properties needed for a light-weight structural material. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% Mg while the most ductile alloys have 0-20 at.% Mg. An Ashby map containing Y/ρ vs. B/G shows that it is not possible to increase both Y/ρ and B/G by changing only the composition of a binary alloy (W. A. Counts, M. Friák, D. Raabe, J. Neugebauer, Acta Mater 57 (2009) 69).

MM 5.2 Mon 10:30 IFW D

Effect of interstitial carbon on the magnetic structure of fcc iron: Towards an ab-initio understanding of austenitic steels — •Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH,Max-Planck-Straße 1,40237 Düsseldorf,Germany

It is known that the mechanical properties of austenitic steels strongly depend on their carbon content. However, the impact of carbon on the stability of the complex magnetic structure of the austenitic iron host is still controversially debated in the literature. Therefore, we present a systematic ab initio investigation of the interaction of interstitial C with the magnetic structure of austenitic iron. Our results are obtained within the DFT-GGA approach, making use of the PAW method and the collinear approximation for the magnetic moments. We find a principle preference of the C atoms for a FM environment. However, this yields only for very high carbon concentrations (>10 at.%) to a preference of the FM structure for the entire austenitic crystal. For lower concentrations (< 3 at.%), the anti-ferromagnetic double layer (AFMD) structure, representing the magnetic ground-state of pure fcc-Fe, remains the most stable phase. The transition from AFMD to FM ordering takes place at 8 at %, is surprisingly sharp, and a collective phenomenon of all C atoms in the Fe host matrix.

MM 5.3 Mon 10:45 IFW D

DFT calculations on the Fe/ZrO2 system — •Kutzner Jürgen and Kortus Jens — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

The interface Fe/ZrO_2 has been investigated in view of its interface structure and mechanic properties by means of density functional theory calculations.
The pure phases of iron and zirconium dioxide have been studied first as point of reference. The results include phase transitions and bulk-moduli which compare well with experimental data. Further, we have examined possible structural models of simple epitactic phases of Fe and ZrO_2. These models will be discussed in terms of their relative stability. At a next step iron is replaced by more realistic approximations of steel. The influence of different chemical composition on interface structure and materials properties is investigated.
We would like to thank the DFG for financial support within SFB 799: TRIP-Matrix-Composite.

MM 5.4 Mon 11:00 IFW D

The free energy of iron: Integrated ab initio derivation of vibrational, electronic, and magnetic contributions — •Fritz Körmann, Alexey Dick, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

In this talk we present our recently developed [1] integrated ab initio approach including vibrational, electronic, and magnetic contributions to derive the thermodynamic properties of ferromagnetic bcc iron. The quasiharmonic approximation and finite-temperature density functional theory are employed to account for vibrational and electronic excitations. In particular the magnetic contribution to the free energy, which is of crucial importance for the structural phase stability in iron, will be discussed. This contribution has been derived by generalizing an existing many-body theory for the S=1/2 ferromagnet to arbitrary spin quantum numbers and to non-collinear magnetic configurations where the latter is of particular importance for the fcc phase. This approach has lead to an excellent agreement with available experimental data for bcc iron.

[1] F. Körmann, A. Dick, B Grabowski, B. Hallstedt, T. Hickel, and J. Neugebauer, Phys. Rev. B 78, 033102 (2008).

MM 5.5 Mon 11:15 IFW D

Ab initio up to the melting point: Anharmonicity and vacancies in aluminum — •Blazej Grabowski, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Düsseldorf, Deutschland

At elevated temperatures, the heat capacity of metals strongly deviates from the harmonic prediction. This was pointed out long ago[1] and various explanations have been considered. Recently, *ab initio* calculations showed that a dominant part can be explained by quasiharmonic and electronic excitations.[2] However, the *detailed* balance of further contributions, such as explicit anharmonicity and vacancies, is not clarified yet even for simple elementary metals. Aluminum is a prototypical example. Even though intensively studied, the ambiguous experimental situation has made a classification of the mechanisms impossible.

To resolve the situation, we have calculated the full volume and temperature dependent *ab initio* free energy surface employing density-functional theory. In particular, we have included anharmonic and vacancy contributions using numerically highly efficient methods to coarse grain the configuration space. To obtain accurate vacancy energies, we have included the full spectrum of excitations: quasiharmonic, electronic, and explicitly anharmonic. The results are in contradiction to common belief, nevertheless the essential physics can be captured by a simple model.

1. M. Born and E. Brody, Zeitschrift für Physik 6, 132 (1921).
2. B. Grabowski, T. Hickel, and J. Neugebauer, Phys. Rev. B 76, 24309 (2007).

MM 5.6 Mon 11:30 IFW D

Theoretical multi-physics approaches to solid-solution strengthening of Al — •Duancheng Ma, Martin Friák, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The strengthening of soft metallic materials has a long tradition and is an important metallurgical topic since the time when ancient smiths forged the first swords. Intense materials research revealed a combination of three mechanisms as decisive for solid-solution strengthening phenomena: (i) the size mismatch of components (Mott and Nabarro's parelastic concept [1]), (ii) the elastic modulus mismatch of atoms (Fleischer's dielastic contribution [2]), and (iii) the concentration of solutes (statistical concept of Friedel [3] and Labusch [4]). Combining density functional theory calculations and linear-elasticity theory, the key parameters that are essential for the classical strengthening theories are determined in order to test them and identify their possible validity limits. The strengthening of fcc aluminium is chosen as an example and a series of binary systems Al-X (with X = Ca, Sr, Ir, Li, Mg, Cu) was considered. Comparing our results with those obtained by applying classical theories we find clear deviations. These deviations originate from non-classical lattice distortions due to the size mismatch of solute atoms in their first coordination shells.

1. N. F. Mott and F. R. N. Nabarro, Proc. Phys. Soc. **52**, 86 (1940).
2. R. L. Fleischer, Acta. Metall. **9**, 996 (1961).
3. J. Friedel, Dislocations (1964).

4. R. Labusch, Phys. Stat. Sol. **41**, 659 (1970).

MM 6: Materials Design II

Time: Monday 12:00–13:00 Location: IFW D

MM 6.1 Mon 12:00 IFW D

Application of evolutionary strategies to crystal structure prediction — •Silvia Schumann and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09599 Freiberg, Germany

This work presents first tests of an evolution strategy for crystal structure prediction. For evaluation we chose elements of the third main group of the periodic system of elements, excluding boron. The crystal structures of these elements at ambient pressure are well known and have been selected because they have considerably different space groups, despite their same isovalent electronic structure and their similar chemistry.

For the evolution strategy a randomly chosen population of lattices is evaluated using pseudo-potentials to compute the free energy of each lattice. The more stable (lowest free energy) lattices are allowed to recombine and are mutated to form the lattices of the next generation. Contrary to conventional minimization methods the evolution strategy avoids trapping in local minima and provides a wide-range search of the high-dimensional search space. Possible slow convergence rates of evolution strategies close to minima are countered by applying conventional structure relaxation.

MM 6.2 Mon 12:15 IFW D

Structure formation described in terms of General Dynamics instead of Thermodynamics only — •Peter Häussler — Chemnitz University of Technology, Institut of Physics, 09107 Chemnitz

Phase formation is still not well understood. Generally, it is described in terms of thermodynamics under the influence of *external* parameters as e.g. volume V, temperature T, and concentration x, if alloys are described. Microscopically, by applying quantum mechanics, phase formation is described by Schrödinger's equation, dealing with *internal* quantities as the momentum $\vec{p}$, and/or angular momentum $\vec{L}$. Subsequently, till the present, there is a gap between both descriptions.

In recent contributions we were able to show that phase formation is strongly dominated by self-organizing resonances between global *internal* subsystems, causing gaps or pseudogaps at the Fermi energy of the electronic states (Peierls-, Hume-Rothery-like). The self-organization is based on an exchange of momentum and angular momentum, neither described by the present thermodynamics, nor by Schrödinger's equation as long as Bloch's theorem can not be applied (as soon the system is still without strict periodicity). We implement the internal effects between global subsystems to a description of phase formation in terms of Gibbs General Dynamics instead of Thermodynamics only. During structure formation, going from the anti-bonding resonant state to the bonding one, entropy is created, allowing the total system to release as much energy as possible.

MM 6.3 Mon 12:30 IFW D

Entwicklung einer Messmethode zur Bestimmung der Auflösung und ihrer Verifikation an einem Au/PtRu-System — •Alexander Schökel und Christina Roth — TU Darmstadt, Deutschland

Bei dem für Brennstoffzellen etablierten Katalysatorensystem PtRu kommt es im Direktmethanolbetrieb zu einer Auflösung des Ru. Dies führt zu einer Degradation der Brennstoffzelle. Untersuchungen durch Liang et al. [1] haben gezeigt, dass durch Deposition von Au-Nanopartikeln das Oxidationspotential von Ru erhöht wird und sich das Ru so gegen seine Auflösung stabilisieren lässt. Neben Au kommen auch andere Elemente für solche ternäre Katalysatorensysteme in Betracht. Theoretische Modellierungen sollen solche Kandidaten identifizieren. Katalysatorsysteme, die sich in experimentellen Untersuchungen als aussichtsreich erweisen, werden danach in Modell- und Prototypenzellen weiter untersucht.

Die TU Darmstadt entwickelt derzeit quantitative Methoden, mit deren Hilfe der Grad der Ru-Auflösung möglichst unter beschleunigten Alterungsbedingungen bestimmt werden kann. Die Entwicklung dieser Methoden und ihre Verifikation am Beispiel eines Au/PtRu-Systems sollen hier vorgestellt werden.

[1] Z.X. Liang, T.S. Zhao, J.B. Xu, J. of Power Sources 185 (2008) 166-170

MM 6.4 Mon 12:45 IFW D

Differential phase contrast setup for a non coherent beamline at HASYLAB using hard x-ray grating interferometer — •Julia Herzen[1], Felix Beckmann[1], Tilman Donath[2], Christian David[2], Franz Pfeiffer[2,3], Christian Grünzweig[2], Astrid Haibel[1], and Andreas Schreyer[1] — [1]GKSS Research Centre, Geesthacht, Germany — [2]Paul Scherrer Institute, Villigen PSI, Switzerland — [3]EPF Lausanne, Lausanne, Switzerland

Phase-contrast imaging is a common technique to visualize soft tissue with much higher contrast than the conventional absorption-contrast imaging. Differential phase contrast (DPC), developed at PSI, Switzerland, makes use of a hard x-ray grating interferometer and allows for phase-contrast imaging with high brilliance synchrotron sources as well as with conventional x-ray tubes. It is recently reported also to provide dark field information that is very sensitive to micro structures like porosity within the materials [1]. Here we present the plans to adopt the DPC technique to the HARWI-II materials science beamline [2], operated by GKSS Research Centre, in cooperation with DESY, Hamburg. This will offer an amount of new applications especially in the field of materials science like for example characterizing new light weight materials like magnesium and studying its corrosion as implant material. [1] F. Pfeiffer, M. Bech, O.Bunk, P. Kraft, E. F. Eikenberry, CH. Brönnimann, C. Grünzweig, and C. David, Nature Materials 7, pp.134-137 (2008). [2] F. Beckmann, T. Donath, J. Fischer, T. Dose, T. Lippmann, L. Lottermoser, R. V. Martins, and A. Schreyer, Proc. of SPIE Vol. 6318, 631810 (2006).

MM 7: HV Hofmann

Time: Monday 14:00–14:30 Location: IFW A

Invited Talk MM 7.1 Mon 14:00 IFW A

Non-destructive residual stress analysis with neutrons — •Michael Hofmann — FRM II, TU München, Garching, Germany

The measurement and analysis of residual stresses has gained significant importance over the past couple of years due to the increasing demands in improving the properties of new engineering materials and components. The ability to measure these residual stresses accurately will thus lead to the manufacture of stronger, lighter and cheaper components by industry. The drive to optimise material performance whilst minimising component weight will ensure that this field continues to grow. Experimentally, non-destructive analysis of phase specific residual stresses is only possible by means of diffraction methods. While X-ray scattering is essentially a surface method, the high penetration depth of neutrons into the bulk material (e.g. 20 mm into steel or 100 mm into aluminium) allows to extract reliable information from within components. In future, neutron scattering will gain further importance for strain measurements as new dedicated neutron diffractometers with advanced neutron optics become available. These will allow the utilization of the full potential of the technique and will help to establish neutron stress analysis as a routine method for industry.

MM 8: Topical Session Nanoporous Functional Materials III

Time: Monday 14:45–16:30 Location: IFW A

Topical Talk MM 8.1 Mon 14:45 IFW A

Geordnetes nanoporöses Aluminiumoxid: Ein vielseitiges Templatsystem — •Ulrich Gösele — MPI für Mikrostrukturforschung, Halle

Elektrochemisch hergestelltes anodischen Aluminiumoxid mit zweidimensionalen geordneten Nanoporen hat sich zu einem der vielseitigsten Templatsysteme für die Nanotechnologie entwickelt. Mit relativ geringem Aufwand lassen sich diese geordneten Nanostrukturen aus Aluminiumoxid mit verschiedenen Porendurchmessern und Abständen erzeugen. Die Porenstrukturen können dann mit verschiedensten Methoden entweder mit bestimmten Materialien gefüllt werden, was zu Nanodrähten führt, oder aber beschichtet werden, was Nanoröhren ergibt. Es wird auf neuere Entwicklungen der Herstellung mittels der sogenannten harten Anodisation eingegangen, die es erlauben, geordnete Strukturen wesentlich schneller als mit der üblichen milden Anodisation und mit einer gezielten Variation des Porendurchmessers herzustellen. Ultradünne poröse Aluminiummembranen können als Masken für die Herstellung geordneter Nanostrukturen verwendet werden, wie z. B. für vertikale einkristalline Siliziumnanodrähte mit Durchmessern unter 10 nm oder für ferroelektrische Nanokondensatoren für die Datenspeicherung.

Der Beitrag beruht auf veröffentlichten Forschungsergebnissen aus dem MPI-Halle, die in Zusammenarbeit mit zahlreichen Doktoranden, Postdocs und Mitarbeiterinnen erzielt wurden, denen ich hiermit herzlich danke. Besonders hervorgehoben seien hier nur Frank Müller, Kornelius Nielsch, Martin Steinhart, Woo Lee und Liufeng Liu.

Topical Talk MM 8.2 Mon 15:15 IFW A

Porous silicon as functionalized magnetic material — •Heinz Krenn, Klemens Rumpf und Petra Granitzer — Institut für Physik, Bereich Experimentalphysik, Karl-Franzens-Universität Graz

Porous silicon prepared as a template for 1D wires or as 3D particles is increasingly used for gas testing, micro devices, batteries and for biological testing equipment. The focus of the present study will be on magnetic functionalization: The electrochemical synthesis of mesoporous silicon allows tailored pore sizes for a controllable inclusion of magnetic transistion metals (Ni, Co). The corresponding spin magnetism is well understood for magnetic fields below 1 Tesla. Interestingly for high fields ($>$ 3T) a novel kind of orbital magnetism [1] is observed mediated by spin injection from the metal into the silicon matrix (which is still crystalline) driven by impurity assisted tunneling. In the same way as electrochemical etching is self-limited by forming a depletion layer, the silicon matrix becomes intrinsic. Due to quantum and dielectric confinement the energy levels of ionized impurities are blue-shifted. If these levels are resonant with the Fermi-level of Ni or Co wire, unbalanced spins are injected and persistent currents around the wires cause orbital paramagnetism in the symmetry-breaking electric field of the interface barrier. Strange effects are observed: negative magnetization in the hysteresis loop, non-saturation up to 7 T, and suppression of orbital magnetism under cyclotron resonance conditions. [1] K. Rumpf, P. Granitzer, H. Krenn, J. Phys.: Condens. Matter 20 (2008) 454221. (Work supported by the Austrian Science Fund under grant P18593).

Topical Talk MM 8.3 Mon 15:45 IFW A

Nanoporous gold: surface chemistry and catalysis — •Marcus Bäumer — Institut für Angewandte und Physikalische Chemie, Universität Bremen, Germany

Nanoporous gold (npAu) is a material with remarkable surface chemical properties. Recently, we found out that it catalyzes low temperature CO oxidation without meeting the requirements usually considered to be important for gold catalysts (small particle sizes, oxide supports). Moreover, we could show that is a promising catalyst for the selective oxidation of alcohols. For the latter reaction the results are in full agreement to UHV studies on gold single crystal surfaces [1] proving that such model systems allow elucidating details of the surface chemistry of npAu at the atomic level. Another interesting feature of the material is the high surface-to-volume ratio resulting in macroscopic length changes as a response of reactions taking place on the surface of the porous structure. Apart from these applications, also the role of residual silver in the material and the question whether a bimetallic surface composition is important for the observed phenomena will be addressed. (The following collaborations are acknowledged: J. Biener/A. Hamza, Lawrence Livermore Nat. Lab.; C. Friend/R.J. Madix, Harvard University; J. Weissmüller, INT FZ Karlsruhe; M. Gottfried, H.-P. Steinrück, Univ. Erlangen) [1] R.J. Madix et al., J. Catal. 258 (2008) 410.

MM 8.4 Mon 16:15 IFW A

Electrochemically-gated field-effect transistor with Indium Tin Oxide nanoparticles as active layer — •Subho Dasgupta, Robert Kruk, and Horst Hahn — Institute for Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany

We report a Field Effect Transistor (FET) device with a Transparent Conducting Oxide (TCO) nanoparticle channel, using solid electrolyte as a gate [1]. FETs in the nanometer scale require channel conductivities as high as possible, therefore, a conductor like Indium Tin Oxide (ITO) was chosen as an active element. ITO nanoparticles were used in order to maximize the active surface area. In the present work, the device principle is based on the variation of the drain current induced by the capacitive double layer charging at the electrolyte/nanoparticle interfaces. The device with metallic conducting channel made of ITO nanoparticles exhibits an on/off ratio of 2×10^3 even when the gate potential is limited within the electrochemical capacitive region to avoid redox reactions at the interface. The field-effect mobility is calculated to be 24.3 cm^2/Vs which exceeds the values reported earlier for the PbSe and In_2O_3 nanocrystalline channel FETs. A subthreshold swing between 230-425 mV/decade is observed.

[1] S. Dasgupta, S. Gottschalk, R. Kruk, H. Hahn, Nanotechnology 19, 435203 (2008)

MM 9: Intermetallic Phases I

Time: Monday 14:45–15:45 Location: IFW B

MM 9.1 Mon 14:45 IFW B

Ab-initio based study of antisite-precipitates in B2-CoAl — •Nils Schindzielorz and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudstr. 7 D-91058 Erlangen

It is well-known that for high temperatures around 1500K the B2-phase of CoAl up to about 70% Co is stabilized by the existence of so called antisite atoms [1]. By quenching the crystal to low temperatures, this phase separates into an ideal B2-CoAl crystal and precipitates consisting of Co antisites only. By the combination of a density functional theory based cluster expansion Hamiltonian with Monte-Carlo simulations it will be demonstrated that these Co clusters show a characteristic size-shape-temperature dependence. Furthermore, we find a flattening of the precipitates at low temperatures due to the anisotropy of the interfacial energy which is wiped out at higher temperature by entropy. A detailed knowledge of the structure of these nanoclusters is of special importance as they lead to local magnetism in a non-magnetic intermetallic compound.

Supported by Deutsche Forschungsgemeinschaft.

[1] V. Blum et al., Phys. Rev. Lett. 89, 266102 (2002)

MM 9.2 Mon 15:00 IFW B

Effective potentials for rhenium in Ni–Al superalloys — •Peter Brommer[1,2], Stefano Angioletti-Uberti[2], and Mike Finnis[2] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [2]Thomas Young Centre, Imperial College, London, UK

It is widely believed that rhenium, which is commonly used in alloys for

turbine blades, is important in increasing the creep resistance of nickel-based superalloys, but the exact reason for this so-called "rhenium-effect" remains unclear.

Atomistic simulations could help study the influence of rhenium on the mechanical properties and compare it to that of other alloying elements. These simulations require effective interaction potentials, as only with those the required large number of particles can be studied. We generated rhenium interaction potentials with the force matching method, where the parameters of a potential are adjusted to optimally reproduce the forces, energies and stresses in a number of reference configurations, which have been evaluated with first-principles density functional theory (DFT) methods.

We use these potentials to study self-diffusion coefficients in liquid and solid alloy phases and compare the results to ab-initio data.

MM 9.3 Mon 15:15 IFW B

Structural stability of topologically close-packed phases in transition metals — •Thomas Hammerschmidt[1], Bernhard Seiser[2], Ralf Drautz[1], and David G. Pettifor[2] — [1]ICAMS, Ruhr-University Bochum, Bochum, Germany — [2]Department of Materials, University of Oxford, Oxford, UK

The formation of topologically close-packed (tcp) phases in Ni-based superalloys leads to the degradation of the creep properties of the alloys. The precipitation of the tcp phases is attributed to refractory elements that are added in low concentration to improve creep resistance. We have compiled a structure map of the occurrence of tcp phases in binary transition metal (TM) compounds. The structure map displays well-established structural trends that are driven by the d-band filling. It also shows that different sizes of the elements tend to stabilize the Laves phases over other tcp phases. The same trend is reproduced in our extensive density functional theory (DFT) calculations of the tcp phases A15, C14, C15, C36, μ, σ, and χ. We show that the structural trend can be understood using the canonical d-band tight-binding model. The small positive values of the heats of formation of all tcp phases suggest that entropy plays a key role in the stabilization of the experimentally observed tcp phases in TM binary compounds.

MM 9.4 Mon 15:30 IFW B

Structural trends in topologically close-packed phases — •Bernhard Seiser[1], Thomas Hammerschmidt[2], Ralf Drautz[2], and David Pettifor[1] — [1]Department of Materials, University of Oxford, Oxford, UK — [2]ICAMS, Ruhr-University Bochum, Bochum, Germany

The creep properties of modern single-crystal Nickel-base superalloys are improved by adding refractory elements. This route of material design is limited by the precipitation of topologically close-packed (tcp) phases which can lead to failure during service. We have assessed the modelling techniques PHACOMP and CALPHAD which are commonly used to predict the tendency of tcp phase formation in austenitic alloys. Moreover, within a tight-binding framework, we have derived analytic bond-order potentials (BOP) that depend explicitly on the valence of the transition metal elements. In particular, we applied these BOPs to investigate the structural stability of tcp phases with respect to the filling of the d-band. From these BOP calculations, we find two groups of tcp phases that exhibit very similar dependence on the d-band filling: A15 and σ on one hand and μ and the Laves phases C14, C15, C36 on the other hand. Through the BOPs we have been able to unravel the link between structural stability and local topology and have identified the interactions that favour the formation of tcp phases.

MM 10: Intermetallic Phases II

Time: Monday 16:00–16:45 Location: IFW B

MM 10.1 Mon 16:00 IFW B

Ordering and site occupancy of ternary elements in Fe_3Al — •Thomas Rademacher, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Ordered iron aluminides exhibit a number of advantageous properties, such as high-temperature strength, corrosion resistance and low cost. Therefore, iron aluminum based alloys are considered to replace in some cases high alloyed ferritic stainless steels, especially DO_3 - ordered Fe_3Al. The mechanical properties and high-temperature stability can be optimized when ternary elements are added.

In this study the site occupancy of ternary elements (4at.%V, 5at.%Cr, 5at.%Mn) has been investigated by means of Atom Probe Tomography (APT). A special analysis algorithm allows resolving the atom layers for different measurement directions which enables determining site preferences. Additionally, comparing the succession of layers with simulations the binding energies of the participating elements can be estimated.

MM 10.2 Mon 16:15 IFW B

Structural interrelations between cubic icosahedral approximants of the Ru-Sb-Zn system — •Bernd Harbrecht and Ding-Bang Xiong — Department of Chemistry, Centre of Materials Science, Philipps University, 35032 Marburg, Germany

Structural complexity in intermetallics comes in different guises, often not just as one phase rather than - as result of small energy differences between compositionally and structurally intimately related phases - in bundles of phases. Positional and substitution disorder may be one cause, long-range vacancy ordering another [1]. More attention has been paid recently to (in)commensurately complex alloy structures, quasicrystals QCs, and quasicrystal approximants QCAs, in which unusual rotational symmetries are relinquished that usual 3D translation symmetry can guide matter to the state of rest. We will present new examples of QCAs we found in the Ru-Zn-Sb system by partly substituting Sb for Zn and Ru in Ru13-δZn128-δ* (hP564-4(δ-δ*)[2], yielding icosahedral approximants of idealised composition Ru26Sb24Zn67 (cF936), Ru13Sb12Zn81, and Ru13Sb6Zn87 (cF848), homotypic to Mo7Zn40Sn12 [3]. The structures will be discussed in the light of the hierarchical approach by decorating high symmetry points with clusters instead with atoms, here with double-Mackay M127 and M119 snub cube clusters with and without additional glue atoms.

[1] S. Thimmaiah, B. Harbrecht, J. Alloys Comp. 2006, 417, 45. [2] C. Allio, B. Harbrecht, Z. Anorg. Allg. Chem. 2006, 632, 2142. [3] H. Hillebrecht, V. Kuntze, K. Gebhardt, Z. Kristallogr. 1997, 212, 840.

MM 10.3 Mon 16:30 IFW B

Characterization of MAX phases via hyperfine interactions — •Daniel Jürgens[1], Michael Uhrmacher[1], Hans Hofsäss[1], Agnieszka Kulinska[1,2], Jose Mestnik Filho[3], and Michel Barsoum[4] — [1]II. Physikalisches Institut, Universität Göttingen, 37073 Göttingen, Germany — [2]IFJ PAN, 31-342 Krakow, Poland — [3]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 Sao Paulo, Brazil — [4]Dep. Mat. Science and Eng. Drexel University, Philadelphia, PA 19104, USA

$M_{n+1}AX_n$ phases, where n is 1, 2 or 3, are nanolaminated layered ternary carbides and nitrides, which feature a unique combination of the best attributes of both metals and high-performance ceramics. This class of solids possesses good electrical and thermal conductivities as well as high thermal shock resistance and damage tolerance.

The method of perturbed angular correlation (PAC), which is sensitive to hyperfine interactions, is used for material characterization on microscopic scale. ^{111}In was implanted as probe nuclei to measure the electric field gradients (EFG) in the *key-compounds* Ti_2InC and Zr_2InC to determine strength and symmetry of the EFG on the In-site or more general on the A-site. Regarding to the question of lattice location of In-probes in In-free MAX phases, PAC studies of Ti_2AlN and Cr_2GeC were performed to confirm the assumption occupying the A-site. The experimental results are compared with those from *ab initio* calculations using the FP-LAPW+LO method implemented in the WIEN2k code. Additionally investigations of annealing behavior, thermal stability and behavior under isostatic stresses are presented.

MM 11: Growth

Time: Monday 14:45–16:15 Location: IFW D

MM 11.1 Mon 14:45 IFW D

Tales of the abnormal: nanocrystalline grain growth at low temperatures — •Heiko Paul and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Unlike in coarse-grained polycrystalline materials, which manifest grain-boundary-controlled growth kinetics, nanocrystalline specimens are presumed to exhibit a coarsening behavior that is affected by their high number density of triple junctions and quadruple points. The consequences of such microstructural features on the nature of grain growth are potentially complex and still not well understood, but most current grain-growth models predict that the rate-controlling mechanism depends on the average grain size, with the dependence extending to larger sizes at lower annealing temperatures. Using a combination of x-ray diffractometry and electron microscopy, we have investigated the low-temperature evolution of microstructure in nanocrystalline Fe prepared by ball milling. The initial stage of grain growth agrees qualitatively with models positing a transition from triple-junction-controlled boundary migration to the standard grain-boundary-controlled case, but a quantitative examination of various moments of the grain-size distribution points to a different explanation: the samples appear to coarsen abnormally at first but to resume a normal growth mode at larger average grain sizes. The striking similarity of this behavior to the room-temperature growth observed in nanocrystalline Pd [1] suggests that abnormal grain growth may not be so "abnormal" after all!

[1] M. Ames *et al., Acta mater.* **56** (2008) 4255–4266.

MM 11.2 Mon 15:00 IFW D

Potts model simulation of triple junction limited grain growth — •Dana Zöllner and Peter Streitenberger — Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

The size effect observed for nanocrystalline grain growth can be attributed to a limited grain boundary junction mobility yielding a junction drag.

Two different approaches are considered in the Monte Carlo Potts model: for one an effective mobility can be introduced, which is reduced by the triple junction distance and secondly each grain feature (grain boundary, triple line and quadruple points) can be assigned an own mobility. These changes in the mobility can be implemented in the Potts model through the transition probability, which calculates the attempted orientation change.

Some results of these modified Potts model simulations will be presented especially regarding the temporal development of the mean grain size and the grain size distribution. It will be shown that for the 2D case for initially very small grains a linear grain growth kinetics is observed followed by a transient state, which in later stages becomes parabolic. Furthermore, in the linear growth regime a coarsening state is reached, where the grain size distributions are shifted to smaller relative grain sizes. The coincidence of the scaled distributions implies the existence of a temporarily universal grain size distribution, which is in agreement with theoretical results based on a grain size dependent boundary mobility.

MM 11.3 Mon 15:15 IFW D

Phase-field simulations in peritectic system — •guillaume Boussinot, efim Brener, and dmitri Temkin — IFF-th.3, Forshungszentrum Juelich, Germany

We use a multi-phase-field model, to study peritectic systems in the case of isothermal processes (where the temperature T of the sample is a given). The latter provide the limit case of directional transformations (where the sample is pulled in a temperature gradient) when the temperature gradient vanishes. When T<Tp, we have a (delta+L-> delta+gamma+L) transformation, where delta is called primary solid phase and gamma is the peritectic solid phase (and L is the liquid). When T>Tp, we obtain a (gamma+L -> delta+L) transformation occuring via a liquid film migration process.

MM 11.4 Mon 15:30 IFW D

Pattern formation during Diffusion limited Transformations in Solids — •Michael Fleck[1], Claas Hüter[1], Denis Pilipenko[1], Robert Spatschek[1,2], and Efim Brener[1] — [1]Institut für Festkörperforschung, Forschungszentrum 52425 Jülich — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum

Key feature of many metallurgical procedures to improve materials properties is the formation of very complex microstructures due to solid-solid phase transformation processes.

We develop a description of diffusion limited growth in solid-solid transformations, which are strongly influenced by elastic effects. Density differences and structural transformations provoke stresses at interfaces, which affect the phase equilibrium conditions. We formulate equations for the interface kinetics similar to dendritic growth and study the growth of a stable phase from a metastable solid in both a channel geometry and in free space. We perform sharp interface calculations based on Green's function methods and phase field simulations, supplemented by analytical investigations.

For pure dilatational transformations we find a single growing finger with symmetry breaking at higher driving forces, whereas for shear transformations the emergence of twin structures can be favorable. We predict the steady state shapes and propagation velocities, which can be higher than in conventional dendritic growth.

MM 11.5 Mon 15:45 IFW D

Crack growth by surface diffusion in viscoelastic media — Robert Spatschek, Efim Brener, and •Denis Pilipenko — Institut für Festkörperforschung, Forschungszentrum Jülich , D-52428 Jülich

Dissipation plays a central role in fracture, since typically only a small fraction on the elastic energy is used to create the surfaces of the advancing crack. Whereas in brittle materials dissipation takes place mainly close to the crack surfaces, in materials with a more viscous behavior an extended zone of bulk dissipation can form around the crack.

We discuss steady state crack growth in the spirit of a free boundary problem. It turns out that mode I and mode III situations are very different from each other: In particular, mode III exhibits a pronounced transition towards unstable crack growth at higher driving forces, and the behavior close to the Griffith point is determined entirely through crack surface dissipation, whereas in mode I the fracture energy is renormalized due to a remaining finite viscous dissipation. Intermediate mixed-mode scenarios allow steady state crack growth with higher velocities than for pure mode I.

MM 11.6 Mon 16:00 IFW D

Theory of dendritic growth in the presence of lattice strain — Efim A. Brener, •Claas Hüter, and Denis Pilipenko — Institut für Festkörperforschung, Forschungszentrum 52425 Jülich

The need to understand the dominating phenomena during solid-solid transitions as they occur in various processes of industrial relevance is apparent.

Elastic effects as they occur due to lattice strain modify the local equilibrium condition at the solid-solid interface compared to classical dendritic growth. Both, the thermal and the elastic fields are eliminated by Green's function techniques and a closed nonlinear integro-differential equation for the interface is derived. In the case of pure dilatation, the elastic effects lead only to a trivial shift of the transition temperature while in the case of the discussed shear transitions and superposition of these basic lattice strains, dendritic patterns are found even for isotropic surface energy. Of course, the discussed elastic effects also introduce an "effective anisotropy" of the system. However, the physics and structure of selection theory for the two mechanisms, anisotropy of surface energy and elastic effects, are fundamentally different. Elastic effects lead to a much more robust selection mechanism compared to tiny effects of anisotropy of surface energy. Moreover, the growth velocities for the same effective driving force can reach appreciably larger values than in the case of selection via anisotropy of surface energy.

MM 12: HV Dehm

Time: Tuesday 9:30–10:00 Location: IFW A

Invited Talk MM 12.1 Tue 9:30 IFW A

Small scale mechanical testing: Challenges and benefits — •Gerhard Dehm — Erich Schmid Institut für Materialwissenschaft der Österreichische Akademie der Wissenschaften — Department Materialphysik, Montanuniversität Leoben

The continuous trend in miniaturization of materials requires novel strategies to probe the mechanical properties at the micron- and submicron level. Thin film structures, micro- and nanowires, as well as nanostructured materials like in microelectronic devices, flexible electronics, cutting tools, energy systems and high temperature materials are examples were small scale mechanical testing methods are most promising to determine strength and failure mechanisms. This information is needed for a fundamental understanding as well as to guide the development of robust products. Focussed ion beam microscopy and lithography routes are employed to shape quantitative deformation and fracture experiments at small length scales. In situ scanning electron microscopy and transmission electron microscopy as well as advanced X-ray diffraction experiments are combined to get insight in the underlying deformation mechanisms. Some of the challenges encountered in small scale mechanical testing are discussed.

MM 13: Topical Session Nanoanalytics using Small-Angle Scattering I

Time: Tuesday 10:15–11:30 Location: IFW A

Invited Talk MM 13.1 Tue 10:15 IFW A

Small-Angle Neutron Scattering in Materials Science — •Pavel Strunz[1], Debashis Mukherji[2], Gerhard Schumacher[3], Ralph Gilles[4], and Albrecht Wiedenmann[5] — [1]NPI and Research Centre Řež, CZ-25068 Řež near Prague — [2]TU Braunschweig, IfW, Langer Kamp 8, D-38106 Braunschweig — [3]Helmholtz-Zentrum Berlin, Glienicker Str. 100, D-14109 Berlin — [4]TU München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Lichtenbergstr. 1, D-85747 Garching — [5]ILL, 6, rue Jules Horowitz, BP 156, F-38042 Grenoble Cedex 9

A complementary use of Small-Angle Neutron Scattering (SANS) can be considered for microstructural investigations. In special cases, it can even be indispensable as it provides information not accessible by other methods. Due to the low absorption of neutrons by a majority of elements, it is a suitable method for bulk characterization as well as for in-situ studies at extreme conditions. Neutrons enable relatively easy contrast variation which helps to resolve details of microstructure. A sensitivity to magnetic inhomogeneities has to be pointed out as well.

Examples taken from the research of Ni superalloys and ceramic thermal barrier coatings demonstrate the application of in-situ SANS in investigation of high-temperature materials. The evolution of precipitates in Ni-Fe-based superalloy and formation of nanopores in YSZ coating was observed. Another study employs contrast variation for characterisation of nanoparticles produced by extracting precipitates from a bulk alloy. The existence of a core-shell structure of the nanoparticles was confirmed by SANS.

MM 13.2 Tue 10:45 IFW A

In-situ SANS study of domain formation during condensation and evaporation of fluids in SBA-15 — •Maxim Erko[1], Johannes Prass[1], Dirk Wallacher[2], Astrid Brandt[2], and Oskar Paris[1] — [1]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, D-14424 Potsdam, Germany — [2]Helmholtz Centre Berlin, Glienicker Straße 100, D-14109 Berlin, Germany

Ordered mesoporous materials such as SBA-15 are ideal model systems to study the sorption and condensation behaviour of fluids in confined geometry. A particularly interesting question relates to collective phenomena such as the formation of domains of unfilled and filled regions that extend over much larger spatial distances than the typical pore size. We have studied the formation and dissolution of such domains upon condensation and evaporation of contrast matching H2O/D2O and Perfluoropentane (C5F12) in SBA-15 silica with in-situ small angle neutron scattering (SANS), using the DEGAS sorption system at the BENSC neutron facility at Helmholtz Centre Berlin. The SANS data can be modelled by randomly distributed domains of filled and unfilled mesopores on a lattice as described by the classical Laue-scattering. Thus, the SANS data in the capillary condensation / evaporation regime can be fitted by an analytical model with only one free parameter, i.e., the filling fraction of mesopores. The quantitative values of this parameter are compared with the results from the independent volumetric sorption experiment, and the differences are discussed with respect to the metastability of the fluid in the adsorption regime.

MM 13.3 Tue 11:00 IFW A

Analytical Determination of Micellar Nanoreactor Structure by Means of SANS — •Roza Bakeeva[1], Alexandr Kuklin[2], and Vladimir Sopin[1] — [1]Kazan State Technological University, Kazan, Russia — [2]Joined Institute for Nuclear Research, Dubna, Russia

We have studied the reaction of decomposition of toxic phosphorus esters (O-4-nitrophenyl-O,O-dimethyl-tiophosphate) in micellar media, containing compounds with nucleophilic properties (potassium fluoride KF and sodium hydroxide NaOH). These additives are electrolytes and their addition brings about the reducing a surface potential micelles and it is possible to control the changing of size and form of micelles. In this instance micelle is considered as nanoreactor.

The SANS method was used to determine the characteristic parameters of nanoreactors - micelles (radius, shape, aggregation number). Neutron scattering curves were obtained on YuMO small-angle scattering setup (two-detector version), using a high-efficiency neutron pulse source (IBR-2 reactor). The shape of scattering associates (micelles) was determined by Porod invariant and Guinier plot analyses, as well by simulation using the FITTER program package The most appropriate model of a particle is a sphere for system CTAB + D2O, CTAB + KF + D2O and a cylinder for system CTAB + KF + NaOD + D2O.

The obtained data have shown that introduction KF brings about the compression of micelles CTAB, but addition of NaOH stimulates the sphere to cylinder transition that in the significant measure defines a difference in their catalytic characteristics.

MM 13.4 Tue 11:15 IFW A

Lots wife problem in biomineralization: An exploration of colloidal protein-minerals particles with SANS — Alexander Heiss[1,2], Vitaliy Pipich[1], Willi Jahnen-Dechent[2], and •Dietmar Schwahn[1] — [1]IFF des Helmholtz Forschungszentrum Jülich — [2]IBMT der RWTH Aachen

The serum protein fetuin-A is an important inhibitor of calcification in mammals. In vitro experiments using SANS and TEM demonstrated, that fetuin-A mediates the formation of colloidal protein-mineral composites (CPP) in aqueous supersaturated calcium phosphate solutions. Colloidal particles, very similar to those in vitro synthesized secondary CPPs, were also found in ascites from a patient with calcifying peritonitis, a rare clinical complication. Here we show that SANS contrast variation provides detailed information on the topology and the composition of protein-mineral colloids.

Fetuin-A gives rise to a two-stage process of colloid formation. The primary CPPs are spherical and have a diameter of 50 nm, whereas the secondary CPPs have an ellipsoidal shape and a diameter of 200x100 nm. Contrast variation SANS in combination with singular value decomposition technique revealed that the primary CPPs appear as a homogeneous protein-mineral composite whereas the secondary CPPs consist of a compact octacalcium phosphate nucleus covered by a fetuin-A monolayer. Moreover, the analysis of the SANS data indicated that in fact most fetuin-A was still in solution as monomers loaded with calcium and phosphate ions.

MM 14: Topical Session Nanoanalytics using Small-Angle Scattering II

Time: Tuesday 11:45–12:45 Location: IFW A

Invited Talk MM 14.1 Tue 11:45 IFW A

Anomalous small-angle X-ray scattering in material science — •Armin Hoell — Helmholtz-Zentrum Berlin für Materialien und Energie, Glienicker Strasse 100, 14109 Berlin, Germany.

Anomalous small-angle X-ray scattering (ASAXS) is an element-selective method based on the anomalous variation of the atomic scattering factor near absorption edges. Nowadays, ASAXS is a mature technique to analyse nano-structures as well as their chemical composition fluctuation. It is used in physics, chemistry, biology and soft / hard condensed matter. This talk will elaborate the advantages of ASAXS in the analysis of complex materials. In the first part important technical details and strategies to measure ASAXS will be emphasized. In the second part some material science applications are chosen to illustrate different aspects and benefits of ASAXS. While using the relative contrast variation between SAXS curves measured at different energies near below absorption edges of elements containing in the sample the composition fluctuations are derived in a demixed supercooled liquid state of a ZrTiCuNiBe alloy. The method of partial structure functions derived from ASAXS will be explained by way of the example of an AlNiLa alloy. So, in case of Ruthenium/Selenium based catalysts ASAXS allows to determine characteristic length-scales associated with three different structural elements. Furthermore, it will be shown how a simultaneous nonlinear regression method including physical constrains can be used to resolve the nano-structure of a silver-free photochromic glass.

MM 14.2 Tue 12:15 IFW A

Small Angle Scattering by Magnetic Nanoparticles — •Sabrina Disch, Raphaël P. Hermann, Peter Busch, Wiebke F. C. Sager, and Thomas Brückel — Institut für Festkörperforschung JCNS and JARA-FIT, Forschungszentrum Jülich GmbH; 52425 Jülich

Intensive research has been dedicated to magnetic nanostructures, both because of their possible applications, e. g. in medical imaging, catalysis, information storage, and owing to the interest in fundamental understanding of their magnetic properties. Magnetic nanoparticles, compared to bulk materials, show unique physical properties such as superparamagnetism or enhanced anisotropy constants. Very little is known about the magnetization distribution within a single particle and magnetic correlations in ordered arrangements of such nanoparticles. Small-angle scattering is the method of choice for investigating both intraparticular phenomena, such as the magnetization distribution or the spin structure of individual magnetic nanoparticles, and interparticular interactions of such nanoparticles in higher dimensional nanostructures. However, before addressing the problems of magnetization distributions or magnetic interactions between magnetic nanoparticles, the availability and the precise structural characterization of highly monodisperse nanoparticles is required. We developed a micellar synthesis route to cobalt nanoparticles with a narrow size distribution and will present latest advances in synthesis optimization and structural characterization along with recent work on highly monodisperse iron oxide nanospheres and nanocubes, including their deposition on substrates and structural characterization by SAXS and GISAXS.

MM 14.3 Tue 12:30 IFW A

Investigation of multiphase systems by small-angle scattering — •Dragomir Tatchev — Helmholtz Zentrum Berlin, Glienicker Str. 100, 14109 Berlin, Germany and Institute of Physical Chemistry - Bulgarian Academy of Sciences, Acad. G.Bonchev Str., Bl. 11, 1113 Sofia, Bulgaria

The two-phase approximation in small-angle scattering is well known and still dominating the data analysis. The intensity scattered at small angles is proportional to the second power of the difference between the scattering densities of the two phases. Simultaneously, scattering contrast variation techniques are widely used and they obviously target multiphase systems or systems with gradually varying scattering density since if no parasitic scattering contributions are present the scattering contrast variation would only change a proportionality coefficient. However, there are only scarce attempts to generalise the SAS theory for multiphase systems. Here we show that the scattered intensity at small-angles of a multiphase system can be presented as a sum of scattering of two-phase systems and terms describing interference between all pairs of phases. Extracting two-phase scattering patterns, called phase scattering functions, from multiphase samples by contrast variation is possible. These two-phase patterns can be treated with the usual SAS formalism. In the case of anomalous SAXS, the phase scattering functions have significant advantage over the partial structure factors since the later depend on all phases in the sample. The case of gradually varying scattering density is also discussed.

MM 15: Topical Session Nanoporous Functional Materials IV

Time: Tuesday 10:15–11:15 Location: IFW B

Topical Talk MM 15.1 Tue 10:15 IFW B

Fluidics with Nanoporous Solid-State Membranes: From Fundamental Physics to Applied Biology — •Patrick Huber — Faculty of Physics and Mechatronics Engineering, Saarland University, D-66041 Saarbrücken, Germany

Transport of fluids across nanopores plays a crucial role in phenomena ranging from clay swelling, frost heave, oil recovery and catalysis, to colloidal stability, protein folding and transport in cells and tissues. The advent of tailorable nano- and mesoporous membranes, most prominently arrays of carbon nanotube bundles, of silicon, silica and alumina channels, has led to a growing interest in fundamental and applied questions with regard to the transport phenomenology across this kind of nanostructures. After a short introduction into this sub-field of nanofluidics, I will present experiments on pressure-driven and self-propelled (capillarity-driven) transport of fluids in nanochannels and will highlight differences between nanoscopic and macroscopic transport principles. Finally, I will elucidate how protein translocation experiments across artificial nanochannel arrays may allow the exploration of the transport machinery at biomembranes.

MM 15.2 Tue 10:45 IFW B

Crystallization Kinetics Dictate the Molecular Arrangement in Nanochannels — •Anke Henschel, Klaus Knorr, and Patrick Huber — Saarland University, Saarbruecken, Germany

We present an x-ray diffraction study on the crystallization of chain-like molecules (medium length n-alkanes and n-alcohols) in arrays of lined up, tubular silicon and silica channels (mean channel diameters of 10 nm)[1–2].

The samples, prepared by capillary condensation or filling in the liquid state and subsequent cooling below the pore freezing point, exhibit diffraction patterns typical of significant, anisotropic orientation distributions of the pore crystals. The architectural principle common to all observed textures originates in a nano-scale version of the mechanism underlying the Bridgman technique of single crystal growth: Upon solidification of completely filled nanochannels the fastest, and hence dominant growth direction, propagates along the long axes of the channels and thereby dictates a distinct orientational arrangement of the molecular crystals.

(1) A. Henschel, T. Hofmann, P. Huber, K. Knorr, Phys. Rev. E 75, 021607 (2007).

(2) A. Henschel, P. Huber and K. Knorr, Phys. Rev. E 77, 042602 (2008).

MM 15.3 Tue 11:00 IFW B

Electrostatic Doping of Strongly Correlated Systems — •Ajay Kumar Mishra, Azad Darbandi, Robert Kruk, and Horst Hahn — Institute for Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany

We present a study on the tuneable magnetic transitions using electrostatic doping (electrostatic modulation of the carrier density upon

surface charging). In strongly correlated materials, like colossal magnetoresistance compounds (CMR), electrostatic doping can alter fundamental properties of the electronic system by inducing phase transitions.

Since the electrostatic doping is a surface effect a large surface-to-volume ratio is desired to get an appreciable modification of the physical properties. In order to obtain such nanostructures, La1-xSrxMnO3 (LSMO) nanoparticles were synthesized by spray pyrolysis. The microstructure of the as synthesized nanoparticles consists of porous, shell-like structures with a particle size of about 8 nm. The magnetic measurements of nanoparticles show superparamagnetic behavior at room temperature. A controlled post annealing was carried out to bring the ferromagnetic transition slightly above room temperature. The sharp transition and favorable surface-to-volume ratio is reached at annealing temperatures between 800-1100 0C, resulting in grain sizes ranging from 30 to 80 nm. A reversible change of 2 % in magnetization is observed when the charge is applied at the solid-electrolyte interface. The magnetization modulation upon charging is discussed in terms of the reversible electrostatic hole doping.

MM 16: Diffusion and Point Defects I

Time: Tuesday 11:30–12:30 Location: IFW B

MM 16.1 Tue 11:30 IFW B

Diffusion and Crystallization in Magnetron Sputtered SiC Films — •Wolfgang Gruber and Harald Schmidt — TU Clausthal, Institut für Metallurgie, AG Materialphysik

Thin films of amorphous and polycrystalline SiC have a great potential for applications in various branches of technology. For a tailored production of polycrystalline films a understanding of nucleation and growth mechanisms which determine the microstructure are necessary. X-ray diffractometry (XRD) and transmission electron microscopy (TEM) studies on r.f. co-sputtered SiC films yielded a strong dependence of the crystallization rates on the substrate. For single crystalline silicon as a substrate an activation energy of about 4 eV is found for the rate of crystallization. If glassy carbon is used as a substrate the corresponding activation energy is about 9 eV. For a closer investigation of this phenomenon, in this study we investigated films deposited on different substrates with different thickness (100 nm to 1000 nm) and variable composition SiCx. Since self-diffusion plays an important role for crystallization we measured the diffusivities of the constituting elements using isotope enriched heterostructures and secondary ion mass spectrometry (SIMS). Based on the experimental results a model for crystallization kinetics is discussed.

MM 16.2 Tue 11:45 IFW B

Atom Jumps Studied by Coherent Synchrotron Radiation — •Gero Vogl[1], Michael Leitner[1], Bastian Pfau[2], Bogdan Sepiol[1], and Lorenz-Mathias Stadler[1] — [1]Fakultät für Physik der Universität Wien, Austria — [2]BESSY, Berlin, Germany

Measuring the atomic diffusion jump is a fundamental problem in solid state physics. Up to now only measurements involving a limited number of isotopes and in a very limited temperature range were feasible due to the limitations of methods such as quasi-elastic neutron scattering, quasi-elastic Mössbauer spectroscopy or nuclear magnetic resonance.

X-ray photon correlation spectroscopy has the potential to overcome these constraints. We present the first successful implementation of this new technique. We deduce the atomic jump model from the q-dependent relaxation times of diffuse scattering measured at the ESRF and give the activation energy of Au diffusion in CuAu. We predict that the new sources with increased brilliance and high coherence like PETRA or the XFEL will enable determination of the atomic diffusion jump in condensed matter over a wide range.

MM 16.3 Tue 12:00 IFW B

Self-diffusion in Germanium at Low Temperatures — •Erwin Hüger[1], Ursula Titze[2], Dieter Lott[2], Hartmut Bracht[3], Dominique Bougeard[4], Eugene E. Haller[5], and Harald Schmidt[1] — [1]TU Clausthal, Germany — [2]GKSS Forschungszentrum Geesthacht, Germany — [3]Universität Münster, Germany — [4]TU München, Germany — [5]University of California at Berkeley, USA

Self-diffusion in intrinsic single crystalline germanium was investigated between 429 and 596 °C using $^{70}Ge/^{nat}Ge$ isotope multilayers. The diffusivities were determined by neutron reflectometry from the decay of the first and third order Bragg peak. At high temperatures the diffusivities are in excellent agreement with literature data obtained by ion beam sputtering techniques, while considerably smaller diffusion lengths between 0.6 and 4.1 nm were measured. At lower temperatures the accessible range of diffusivities could be expanded to values $D < 1 \times 10^{-25}$ m^2s^{-1} which is three orders of magnitude lower than the values measured by sputtering techniques. Taking into account available data on Ge self-diffusion, the temperature dependence is accurately described over nine orders of magnitude by a single Arrhenius equation. An activation enthalpy of diffusion of (3.13 ± 0.03) eV and a pre-exponential factor of 2.54×10^{-3} m^2s^{-1} for temperatures between 429 and 904 °C are obtained. Single vacancies are considered to prevail self-diffusion in Ge over the whole temperature range.

MM 16.4 Tue 12:15 IFW B

Defect structures in CaF_2 for optical applications — •Stephan Rix[1,2], Marisa Aigner[1], Claudia Felser[2], Martin Letz[1], Ute Natura[3], and Lutz Parthier[3] — [1]Schott AG, Mainz — [2]Johannes Gutenberg-Universität, Mainz — [3]Schott Lithotec, Jena

Single crystal calcium fluoride (CaF_2) is an important lens material for deep-ultraviolet optics used in microlithographic structuring of semiconductors. High radiation densities require an extreme laser-stability of the material. The quality of the material strongly depends on a high purity level. For long exposure times the optical quality of CaF_2 is affected by radiation-induced defect structures, namely F- and H-centers. The migration and agglomeration of these defect structures play an important role in understanding laser-damage processes on a microscopic level. We use ab-initio methods to investigate the stabilization of laser-induced defects by agglomeration or impurities. As stabilization processes involve defect migration, we also focus on diffusion properties of defects. We present a method for the calculation of diffusion barriers, which shows good agreement with experimental results for the F-center with well localized electronic wave functions.

MM 17: Mechanical Properties III

Time: Tuesday 10:15–11:45 Location: IFW D

MM 17.1 Tue 10:15 IFW D

Change of deformation mechanism in nanocrystalline nickel at very low temperatures — •Lutz Hollang, Suhash Ranjan Dey, and Werner Skrotzki — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden

Pure nanocrystalline nickel was produced by pulsed electro-deposition without additives for grain refinement. The average grain size of the material is d(EBSD) = 150 nm and d(XRD) = 25 nm if determined by electron backscatter diffraction (EBSD) and X-ray diffraction (XRD), respectively. Tensile tests with constant deformation rate were performed at temperatures between 4 K and 320 K. The stress-strain curves are parabolic with the ultimate stress strongly decreasing with increasing temperature. Stress relaxation experiments reveal that dislocation interaction governs the plastic behaviour of the material at low temperatures. However, if the stress reaches the threshold of 2400 MPa, as it is the case between 4 K and 9 K, the deformation mode suddenly changes towards 'catastrophic' shear. The shear events are characterized by substantial stress drops accompanied by acoustic

emission. The nature of the shear events will be discussed on the basis of microstructural investigations performed by electron microscopy.

MM 17.2 Tue 10:30 IFW D

Deformation behavior of nanocrystalline Pd and Pd-10 at. % Au alloy investigated by mini-compression test — •Lilia Kurmanaeva[1], Yulia Ivanisenko[1], Jürgen Markmann[2], and Hans-Jörg Fecht[3] — [1]Institute für Nanotechnology (INT), Forschungszentrum Karlsruhe, Karlsruhe, Germany — [2]Universität des Saarlandes, FR7.3 Technische Physik, Saarbrücken, Germany — [3]Institute of Micro and Nanomaterials, University of Ulm, Ulm, Germany

Investigations of mechanical properties of nanocrystalline (nc) materials are still in interest of materials science. The method of inert gas condensation (igc) allows to produce nc samples having uniform equiaxed microstructure with the mean grain size of 5-10 nm, and of very high purity. Here, we present results of the microstructure and mechanical properties investigation of nc as-igc Pd and Pd-10 at. % Au alloy. The specimens' microstructure was analysed by means of XRD and TEM, and mechanical properties were studied in compression tests using a dedicated testing stage for miniature specimens. Conventional compression tests showed that samples demonstrate high stress (the yield strength were 0.95 GPa and 1.12 GPa for as-igc Pd and Pd-10%Au, respectively) with significant ductility. Strain-rate jump compression tests revealed high strain rate sensitivity in nc Pd and Pd-Au alloy, strain rate sensitivity parameter (m) was 0.067 and 0.034, and activation volume was 4 and 7 burgers vectors for Pd and for Pd-10%Au, respectively. The obtained results of mechanical properties and microstructure are discussed.

MM 17.3 Tue 10:45 IFW D

Metals Plasticity: Interrelating Different Levels of Description — •Markus Hütter[1], Miroslav Grmela[2], and Hans Christian Öttinger[1] — [1]ETH Zürich, Department of Materials, Polymer Physics, CH-8093 Zürich, Switzerland — [2]Ecole Polytechnique de Montreal, Montreal, Quebec, Canada H3C 3A7

The behaviour of crystalline metals under applied mechanical load can be described on different levels of description, namely, (i) the microscopic constituent particles, (ii) the dislocations on mesoscopic scales, and (iii) the macroscopic continuum. The most one benefits from these separate pieces of information once they are related to each other. In this contribution, we offer some insight in how to achieve these relations. First, coarse-graining is used to constrain the constitutive relation for plastic flow on the macroscopic scale based on the microscopic dynamics of the constituent particles. However, as this approach does not adequately represent the origin of plastic deformation, in a second step, the mesoscopic level of dislocations and their dynamics are taken into account in due detail by the following steps. A kinetic toy model is introduced that can be interpreted as modelling the dynamics of a single dislocation. In contrast to most approaches in literature, our kinetic toy model describes not only the irreversible (plastic) but also the reversible dynamics of the dislocations. Subsequently, we discuss how the effect of multiple dislocations and the interactions between them, that lead to strain hardening, can be taken into account. Finally, we comment on how our approaches of modelling dislocations can be related to the macroscopic description of elasto-viscoplasticity.

MM 17.4 Tue 11:00 IFW D

Multi-scale phase composites in high strength hypoeutectic FeCo-based alloys with large plasticity — •Ran Li[1], Gang Liu[1], Mihai Stoica[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institut für Komplexe Materialien, P.O. Box 27 01 16, D-01171 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

Near-equiatomic FeCo alloy is a famous conventional magnetic material ideally suitable for the applications of high magnetic flux density such as electromagnetic system in aircraft industry. However, notorious brittleness of this alloy obstructs its industrial application. By controlling rapid-solidification condition and designing multicomponent alloying, we produced a family of FeCo-based multi-scale phase composites with good mechanical properties. Comparing with equiatomic FeCo alloy, the designed alloys exhibit 3-7 times improvement of yield stress and plastic deformation of 3-18 % during compressive test. The structural analysis indicated that fined grains induced by the control of liquid solidification and morphologic construction of multi-scale phase composite endow these alloys with good mechanical properties. Although the alloying slightly decreased the saturation magnetization of resulting alloys, it still remains around 2 T as high as the result of pure iron. Furthermore, the strength and deformation behavior are quantitatively related to the volume fraction and size of the multi-scale phases via modeling, which can give a useful guideline to design this kind of composite alloys.

MM 17.5 Tue 11:15 IFW D

Measurement of mechanical properties for materials of interest in microelectronics using indentation methods: porous low-k dielectric and soft metallic thin films as examples — •Matthias Herrmann and Frank Richter — Institute of Physics, Chemnitz Univ. of Technol., 09107 Chemnitz, Germany

For the characterisation of the mechanical behaviour of bulk and thin film materials, physical quantities like Young's modulus E, Poisson's ratio ν, or yield strength Y are most appropriate and can principally be used for modelling and/or predicting materials under load. In contrast to these quantities, the often used hardness depends on the applied measuring method and is less suited for modelling. However, the determination of these properties is difficult because it is distorted by the influence of the substrate. Additionally, problems can arise when the investigated materials start to plastically deform already at very low loads.

In this contribution, indentation methods have been applied to two such special cases: mesoporous SiO_2 as well as MSQ-based films with porosities of 0.30-0.57 and copper films. To determine their Y and E, e.g. elastic-plastic indentations using spheres and sharp tips have been performed, which were analysed by Pharr's concept of the effective indenter. We found Y values between 75-150 MPa for SiO_2 and MSQ films which decreased with increasing porosity. They indicate a tendency to easily plastically deform. The E of these films were between 1-4 GPa. General difficulties with the measurement of plastically deforming materials are exemplarily discussed for the copper films.

MM 17.6 Tue 11:30 IFW D

Elasticity of Porous Materials with Multicontinuous Microstructure — •Sebastian C. Kapfer[1], Christoph H. Arns[2,3], Klaus R. Mecke[1], Stephen T. Hyde[3], and Gerd E. Schröder-Turk[1] — [1]Friedrich-Alexander-Universität, Erlangen, Germany — [2]University of New South Wales, Sydney, Australia — [3]Australian National University, Canberra, Australia

Porous microstructure models reminiscent of existing biomaterials are derived from minimal surfaces of cubic symmetry. The microstructures are composed of a linear elastic solid and a void phase, both of which are continuous. The effective elastic properties of these structures are calculated using a voxel-based finite element method. It is found that effective bulk and shear moduli of the microstructures can be related to the porosity by a power law with fractional exponent. The exponent is found to depend on the topology of the material. Results of similar functional form have previously been reported by A. P. Roberts and E. J. Garboczi for random porous material models (cf. Proc R Soc Lond A (2002) 458 pp. 1033–1054).

MM 18: Mechanical Properties IV

Time: Tuesday 12:00–13:00 Location: IFW D

MM 18.1 Tue 12:00 IFW D

Vergleich der Erholungskinetik aus Doppelzug- und Spannungsrelaxationsversuchen — •Volker Mohles, Sheila Bhaumik und Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen

Während der Erholung verformter Metalle finden Annihilation und Umordnungsprozesse von Versetzungen statt. Beides reduziert die Härte des Materials leicht; vor allem entscheiden diese Prozesse jedoch darüber, ob und wann das Material rekristallisiert und dabei erheblich weicher wird. Daher ist die Kinetik der Erholung von erheblicher

technischer Bedeutung. Zur experimentellen Ermittlung dieser Kinetik sind diverse Versuchsführungen möglich; drei davon werden in diesem Beitrag anhand der kommerziellen Aluminiumlegierung AA3103 verglichen: Doppelzugversuche mit einer Erholungsphase unter Last (DTL), Doppelzugversuche mit Erholungsphase ohne Last (DTU), und Spannungsrelaxationsversuche (SR). DTL und DTU entsprechen unterschiedlichen Erholungsphasen in der Produktion von z.B. Blechen. Die SR sind eine Möglichkeit, die Erholungskinetik zu messen; sie sind experimentell unaufwendiger als DTL und DTU, aber auch empfindlicher und schwerer auszuwerten. Dies liegt daran, dass die Verformung während der Relaxationsphase in geringem Maße fortschreitet und dabei die Relaxationskurve stark beeinflusst. Kleine Störungen bewirken dabei große Auswirkungen auf die Erholungsdaten. Es wird gezeigt, dass SR bei geeigneter Versuchsführung und Auswertung dennoch als preisgünstiger Ersatz für DTL dienen können. Auch für DTU kann zumindest eine gute Approximation ermittelt werden.

MM 18.2 Tue 12:15 IFW D

Influence of Cu atoms on the mobility of dislocations in Cu-doped Al - an atomistic study. — •Thomas Gnielka[1], Pim Schravendijk[2], Christian Elsässer[2], and Peter Gumbsch[1,2] — [1]Universität Karlsruhe (TH), Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg

The influence of substitutional Cu atoms on the mobility of edge dislocations in Cu-doped Al was investigated by means of molecular dynamics simulations with central-force many-body potentials for interatomic interactions in the binary Al-Cu system. For a random distribution of Cu atoms in a low concentration range (up to 0.4% Cu) the damping coefficient and the critical shear stress for the motion of straight dislocations was analyzed.

Furthermore the interaction of edge dislocations with a Σ3 (111) [1-10] symmetrical tilt grain boundary was studied. Up to an applied strain of 1% no propagation of the dislocations across the boundary was achieved. The underlying structural mechanism will be discussed.

MM 18.3 Tue 12:30 IFW D

Temperature dependence of the stacking fault energy in FeMn alloys: An ab-initio study — •Andrei Reyes-Huamantinco[1], Peter Puschnig[1], Levente Vitos[2], Andrei Ruban[2], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, Department of Materials Physics, University of Leoben, Leoben, Austria — [2]Applied Material Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden

The stacking fault energy in Fe-based austenitic alloys (e.g. steels) is an important microscopic parameter that determines the mechanical hardness of the material. Within the axial interaction model it is possible to estimate the stacking fault energy in an fcc crystal from the free energies of the hcp, dhcp (double hcp) and fcc lattices. The vibrational, electronic and magnetic entropy contributions to the free energy have been assessed theoretically, with emphasis on the correct description of the magnetic entropy, in substitutional FeMn binary alloys. Density-functional theory (DFT), the exact muffin-tin orbitals (EMTO) method and the coherent potential approximation (CPA) have been used to calculate the stacking fault energy in random alloys, where simultaneous chemical and magnetic disorder is present. From the analysis of the stacking fault energies as a function of temperature, it is possible to identify the temperatures and Mn concentrations at which the austenitic (fcc) or else the hcp phase is stabilized. The specific role of the disordered local magnetic moments on the stability of FeMn austenitic alloys has been investigated.

MM 18.4 Tue 12:45 IFW D

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

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

MM 19: HV Beke

Time: Tuesday 14:00–14:30 Location: IFW A

Invited Talk MM 19.1 Tue 14:00 IFW A

Diffusion, interface shifts and solid state reactions in nanoscale — •Dezso L. Beke, Zoltan Erdélyi, Zoltan Balogh, Csaba Cserháti, Gabor A. Langer, and Gabor L. Katona — Department of Solid State Physics, University of Debrecen, 4032 Debrecen, P.O.Box 2., Hungary

In a set of recent papers we have shown that the diffusion asymmetry in diffusion couples (the diffusion coefficient is orders of magnitude larger in one of the parent materials) leads to interesting phenomena: i) Sharp interface remains sharp and shifts with non Fickian (anomalous) kinetics [1-3], ii) originally diffuse interface sharpens even in ideal (completely miscible) systems [4,5], iii) there exists a crossover thickness above which the interface shift turns back to the Fickian behaviour [6], iv) the growth rate of a product of solid state reaction can be linear even if there is no any extra potential barrier present (which is the classical interpretation of the "interface reaction control" for linear kinetics). Further results on the growth kinetics of an initially existing thin AB phase in the A/AB/B diffusion couple as well as on the size of the critical nucleus in the "nucleation and growth" mode will also be presented [7,8].

[1]Z. Erdélyi et al., Surf. Sci. 496,129(2002)
[2] G.L. Katona et al., Phys. Rev. B71, 115432(2004)
[3] Z. Balogh et al., Appl. Phys. Lett. 92,143104(2008)
[4] Z. Erdélyi et al. Phys. Rev. Lett. 89,165901(2002)
[5] Z. Erdélyi et al., Science, 306,1913 2004)
[6] D.L. Beke, Z. Erdélyi: Phys. Rev. B73,035426(2006)
[7] C. Csehati et al., J of Appl.Phys. 104,1(2008)
[8] Z. Erdélyi, et al., submitted to Phys. Rev. Letters.

MM 20: Poster Session I

Time: Tuesday 14:45–16:30 Location: P4

MM 20.1 Tue 14:45 P4

Radiotracer Diffusion of Iron and Phosphorus in Sintered Iron Powders — •Deniz Yüksel, Sergiy Divinski, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Germany

Many technological applications require materials with both, good magnetic properties, e.g. fast change of polarisation and high magnetic saturation, and excellent mechanic properties, i.e. large Vickers hardness and high tensile yield stress, at the same time. A strategy for obtaining such beneficial property combination at reasonable materials costs is based on alloying of iron with phosphorus and silicon. We applied a powder metallurgical route for initial materials synthesis. The metal powders were then compacted and sintered. In order to optimize the sintering process, the diffusion kinetics of iron and par-

ticularly of the alloying elements has to be known. We investigated the diffusion of ^{59}Fe and ^{32}P in sintered Fe-P materials as a function of the sintering parameters. The results are discussed with respect to the applicability of the alloys for magnetic applications.

MM 20.2 Tue 14:45 P4

Schadensvorhersage an vordeformiertem und wechselbelastetem Karbonstahl — •Patrick Eich, Matz Haaks und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Die Vorhersage der Lebensdauer von Bauteilen unter zyklischer Belastung basiert bis heute auf der 150 Jahre alten Wöhlermethode. Ein aussagefähiges Wöhlerdiagramm erfordert Lastzahlen von 10^8 bis 10^9 und eine große Anzahl äquivalenter Proben. Damit ist sie sehr zeit- und kostenintensiv. Die Positronen- Annihilations- Spektroskopie (PAS) bietet eine neue Methode der Schadensvorhersage. Die mikroskopische Ursache der Ermüdung ist die Akkumulation von Gitterfehlern, die selbst bei geringer zyklischer Belastung zum Materialversagen führen kann. Die Defektdichte des Materials kann mithilfe der PAS gemessen werden. Selbst geringe Änderungen der Defektdichte, wie sie zu Beginn der Ermüdung auftreten, lassen sich über die Zerstrahlungsparameter bestimmen und als Vorbote der Ermüdung des Materials heranziehen. Die Zuverlässigkeit dieser Methode konnte für Karbonstahl- und Aluminiumproben mit defektarmem Ausgangszustand bereits gezeigt werden. Da der industrielle Auslieferungszustand eine bestimmte Vorschädigung aufweißt, werden aktuelle Ergebnisse von vordeformierten und anschließend wechselbelasteten Zugproben des Karbonstahls C45E vorgestellt. Die Defektdichte wurde mit der Bonner Positronen Mikrosonde untersucht und als Maß für die Schädigung herangezogen. Die Lebensdauer der Proben konnte dabei bereits aus dem Frühstadium der Ermüdung abgeschätzt werden.

MM 20.3 Tue 14:45 P4

Diffusion of Gold in Lead Investigated by Neutron Activation Analysis — •Dirk Böckmann and Nicolaas Stolwijk — Universität Münster, Institut für Materialphysik, 48149 Münster

Fast impurity diffusion in lead has been extensively studied in the 1960s and 1970s. In this context, Pb:Au served as a prototype system. In particular, it was concluded from measurements of Pb self-diffusion enhancement factors in Pb(Au) alloys that the high Au diffusivity cannot be reconciled with the vacancy mechanism. Alternative models interpreted Au transport in terms of fast moving interstitial-type defects including conventional interstitials Au_i, Au_i-vacancy pairs, or Au-Au diplons (dumbbells), however, without providing convincing evidence. Specifically, the role of substitutional Au_s was not sufficiently clarified. Our experiments aim at identifying the mechanism of Au diffusion in Pb by looking closely at the concentration dependence and time evolution of the Au penetration profiles. To this aim, we utilise the suitability of the Pb:Au system for neutron activation analysis (NAA), which allows for the detection of diffusion profiles on an absolute concentration scale. First results are discussed within the framework of interstitial-substitutional diffusion involving Au_i-Au_s exchange with the aid of vacancies.

MM 20.4 Tue 14:45 P4

Investigation of point defects in the cathode material $LiCoO_2$: first-principles calculations — •Melanie Gröting[1], Peter C. Schmidt[2], and Karsten Albe[1] — [1]Materialwissenschaft, TU Darmstadt, Germany — [2]Physikalische Chemie, TU Darmstadt, Germany

Li_xCoO_2 has been widely used in rechargeable lithium ion batteries for decades. Still, there exists no comprehensive understanding of the mechanisms that contribute to degradation in these batteries. However, in the commercially applied concentration range 1.0>x>0.5 microstructural changes, redox and intercalation reactions with the electrolyte, and particularly point defects in the active material are believed to play an important role in the degradation process. Knowledge of the energetics of different point defects are therefore mandatory in order to understand this material more properly.

In this study we use density-functional theory calculations (DFT) to investigate the thermodynamic stability of Li_xCoO_2 with lithium contents x=1.0, 0.5 and 0.0 with respect to the competing metal oxides. Moreover, the formation energies of several charged point defects in these compounds using the supercell approach are calculated. We take lithium and cobalt vacancies into account, as well as oxygen vacancies and interstitials. Especially the oxygen related defects play an important role, which is also evidenced experimentally by performance improvement on coating of the active material e.g. with alumina. Besides the thermodynamic behavior of the defects also the electronic structures and density of states are examined in order to compare them with XPS data.

MM 20.5 Tue 14:45 P4

Spin-phonon scattering and heat transport in spin ladders — •Christina Seidler and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

We study the spin-phonon dynamics and the heat transport of two-leg spin-1/2 ladders in the presence of a magnetoelastic deformation-potential coupling. In the limit of weak inter-rung exchange we employ a mapping of the spin degrees of freedom to a gas of non-interacting bond-bosons to describe the magnetic excitations. The coupled spin-phonon excitations are derived perturbatively and their spectra will be discussed as a function of momentum, frequency, temperature, system parameters and external magnetic fields. Both optical and acoustical phonons will be considered.

The heat transport will be investigated in the linear-response regime by evaluating the corresponding Kubo integrals. Results for the temperature and the magnetic field dependence of both, the magnetic and phononic heat conductance, will be presented. In particular the effect of the field-induced triplet softening will be regarded.

Our results will be put into the context of the anomalous magnetic heat transport of the spin-ladder compound $Sr_{14}Cu_{24}O_{41}$.

MM 20.6 Tue 14:45 P4

Characterization of the Brittle-to-Ductile Transition in NiAl Single Crystals — •Michael Scharnweber, Carl-Georg Oertel, and Werner Skrotzki — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden

Hard oriented NiAl single crystals (<100> deformation axis) have been deformed in compression above and below the Brittle-to-Ductile Transition Temperature (BDTT). The investigation of slip lines suggests a smooth transition from {112}<111> slip at 550 K to {110}<110> slip at 620 K. However, the results of the compression experiments reveal a rather sharp transition in the temperature range 645 K - 655 K. Below the BDTT an anomalous temperature dependence of the yield stress was observed. The activation enthalpy measured supports the deformation model given by Mills et al. [1] suggested for {110}<110> slip. For comparison, soft oriented single crystals (<110> deformation axis) have been deformed in the same temperature range. The active slip system found was {100}<100> with the faint slip line pattern indicating cross slip. For <110> orientation in the whole temperature range investigated the yield stress decreases with increasing temperature.

[1] M.J. Mills, R. Srinivasan, M.S. Daw, Phil. Mag. A, 77, 801 (1998)

MM 20.7 Tue 14:45 P4

How to apply a simulation of field evaporation of intermetallic phases to extract material parameters — •Torben Boll and Talaat Al-Kassab — Institut für Materialphysik, Georg-August Universität Göttingen, 37077 Göttingen, Friedrich-Hund-Platz 1

In this contribution the authors will present a model of the field evaporation process, which is used to reconstruct 3D AtomProbe Tomography (APT) data. The model is based on the commonly used Müller-Schottky-Method to calculate field evaporation field strengths. The simulations are valid for universal formulation and will be focused towards intermetallic phases, such as $L1_0$-TiAl and $L1_2$-Cu_3Au in this presentation. By comparing the results of the simulations with experimental data with the AtomVicinity algorithm material parameters such as the Cu-Au binding energy, the ionization energy or field evaporation field strengths of the respective species can be estimated. Artifacts that are visible in the experimental APT-data can be explained as well. The AtomVicinity algorithm explores the local environment of the atoms and delivers the site occupation of the different species at the respective sublattice positions.

MM 20.8 Tue 14:45 P4

Analysis of GPB zones of AlMgCu alloys — •Iris Kohlbach[1], Björn Korff[1], Benedikt Klobes[1], Torsten Staab[2], Matz Haaks[1], and Karl Maier[1] — [1]Universität Bonn, HISKP, Nussallee 14-16, 53115 Bonn — [2]Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg

In contrast to the textbook example AlCu, early precipitation stages of AlMgCu alloys are not well understood. The first structures for early

precipitates were proposed by Bagaryatsky in 1952 [1]. He suggested a local atomic order similar to the S-phase. However, this has not been confirmed until today. We studied Guinier-Preston-Bagaryatsky (GPB) zones by a comparison of several experimental und numerical methods. According to Bagaryatsky's original suggestion we calculated total and binding energies of several MgCu structures in the Al-matrix using the ab-initio code SIESTA. Unstable structures having negative binding energies are sorted out. Employing the resulting relaxed coordinates we computed positron annihilation (PAS) parameters and XAFS spectra using the codes DOPPLER and FEFF-8, respectively. These data are finally compared with experimental PAS results obtained in Bonn and XAFS spectra measured at BESSY in Berlin. We will present our suggested structures of early precipitates in AlMgCu alloys and introduce the relevant methods.

[1] Y. Bagaryatsky, Dokl. Akad. Nauk CCCP 1952, Tom 87 No. 4 559-562

MM 20.9 Tue 14:45 P4

Concerning the superstructure of rare earth compounds RE_2PdSi_3 — Julia Dshemuchadse, •Tilmann Leisegang, Robert Mietrach, Matthias Zschornak, Torsten Weissbach, Thomas Führlich, and Dirk C. Meyer — Nachwuchsgruppe Nanostrukturphysik, Institut für Strukturphysik, Technische Universität Dresden, Germany

A commensurately modulated structure of the series of compounds RE_2PdSi_3 (RE = rare earth element) is presented. Accordingly, palladium and silicon atoms exhibit partial ordering on the shared B site of the AlB_2-type basic structure. The superstructure has been extensively studied by means of X-ray diffraction on single crystals and other X-ray techniques. Calculations based on density functional theory are compared with the found structure to clarify remaining disorder on atomic sites of the introduced model. Additionally, X-ray absorption spectroscopy measurements reveal the short-range order of RE and palladium atoms, which is associated with the periodic structure. The impact of absorption on the single crystal diffraction data is analyzed by investigating randomly and spherically shaped single crystals. Using X-ray powder diffraction, a significant part of the RE_2PdSi_3 series is investigated to verify the model's applicability to the whole family of rare earth compounds.

We thank the DFG for financial support within the SFB 463.

MM 20.10 Tue 14:45 P4

X-ray Diffraction Analysis and Metal Physics Modeling of Static Strain Aging and Thermal Dislocation Recovery in the Mechanically Affected Zone of Surface Finished Hardened Steel — •Jürgen Gegner — SKF GmbH, Dept. of Material Physics, Ernst-Sachs-Strasse 5, 97424 Schweinfurt, Germany

After heat treatment, finish machining of the hardened steel represents the last manufacturing step of machine elements. The practically most important operation of grinding is applied to achieve edge zone compressive residual stresses, best surface quality and dimensional accuracy. Metal removal involves high plastic deformation work. Glide and intersection processes raise the density and produce lower energy substructures of dislocations. The temperature and time behavior of post-machining thermal treatment is analyzed on ground and honed martensitic SAE 52100 rolling bearing steel. Microstructure stabilization is reflected in a large XRD line width decrease on the surface. The kinetics is modeled by rate-controlling carbide dissolution as the carbon source for Cottrell-type segregation at dislocations. This static strain aging is verified by the formation of a slight white etching surface layer. The metal physics model is extended to also consider superimposed thermal dislocation recovery. Both effects are separable. In rolling contact fatigue tests under mixed friction running conditions, air reheating of the samples below the tempering temperature, which avoids hardness loss, leads to a significant lifetime increase. Thermal post-treatment after cold working results in similar changes of the XRD line width in the larger mechanically affected edge zone.

MM 20.11 Tue 14:45 P4

Investigation of structure dependent resonances in split-ring resonators by terahertz time-domain spectroscopy — •Stefan Waselikowski, Markus Walther, and Hanspeter Helm — Department of Molecular and Optical Physics, University of Freiburg

Recently metamaterials based on split-ring resonator structures raised considerable interest due to their unprecedented electromagnetic properties [1]. Their behavior is mainly dictated by the interaction of their building blocks with an incident light wave and the associated formation of electric and magnetic resonances. We use terahertz time-domain spectroscopy (THz-TDS) [2] to measure the characteristic resonances in different arrangements of metallic split-ring resonators. By varying the resonator geometry we are able to study both, the structure-dependence of the resonances as well as coupling between individual resonators. Our approach takes advantage of the ability of THz-TDS to measure amplitude and phase of the electric field over a wide spectral bandwidth. Furthermore, due to the relatively large wavelength (1 THz corresponds to λ=300 μm) structures with dimensions on the order of the wavelength can easily be manufactured by standard micro-fabrication techniques.

[1] D. R. Smith, J. B. Pendry, and M. C. K. Wiltshire, Science 305, 788 (2004)
[2] D. Grischkowsky, S. Keiding, M. Vanexter, and C. Fattinger, J. Opt. Soc. Am. B 7, 2006 (1990)

MM 20.12 Tue 14:45 P4

Computational Study of Effective Viscosity using a coupled phase-field and Lattice Boltzmann model — •Ali Aksi, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe, Germany

We use a coupled phase-field and Lattice Boltzmann model to measure the effective viscosity of a fluid containing a distribution of particles. The particles are defined as regions with energy bearing boundaries that may differ in their physical states. A Lattice-Boltzmann method is used to describe the motion of the particles in a flow field. We present 2D and 3D simulation results for different types of domains with different amounts of particles, distributions and volume fractions. We also show simulation results using a compressible and incompressible Lattice Boltzmann model in comparison.

MM 20.13 Tue 14:45 P4

Materials science and reverse bioengineering - Status and potential Applications of the nanofocus endstation of μSAXS-beamline at Petra III — •Christina Krywka[1], Stephan Roth[2], and Martin Müller[3] — [1]Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, D-24098 Kiel — [2]DESY, Notkestraße 85, D-22063 Hamburg — [3]GKSS Forschungszentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht

The new synchrotron Petra III is going be a high-brillance synchrotron radiation source, located on the site of DESY in Hamburg, Germany. For this purpose, the existing Petra storage ring is being refurbished into one of the most brillant x-ray sources worldwide and its completion is scheduled for 2009. The μSAXS-beamline of Petra III will be equipped with an additional endstation, designated to provide a high flux x-ray beam focused to about 100nm × 100nm. At the nanofocus endstation experiments with a superior spatial resolution will become available with a flux sufficiently high to study both biological and synthetic materials. This contribution presents an overview on the beamline extension and the current status of its completion. Also, exemplary and potential applications of nanofocused x-rays are shown. Among these are diffraction methods used for the structure determination of synthetic materials (e.g. metallurgy, surface science, semiconductor technology) and biological materials with multiple levels of structural hierarchy (e.g. wood, fibres, cells).

MM 20.14 Tue 14:45 P4

Utilization of thermodynamic databases for phasefield-simulations — •Sebastian Schulz, Abhik Choudhury, and Britta Nestler — Institute of Computational Engineering, Karlsruhe, Germany

To get significant results out of phasefield-simulations, precise thermodynamic properties of the system to be investigated are required as input values. Those values often have to be read out of phase diagrams and typed into the input file manually. An alternative would be the automatic access on thermodynamic databases and their utilization with the Calphad method. In this contribution we intend to present a coupling of thermodynamic databases to the PACE 3D simulation software and the thereby achieved results from simulations of the aluminium/copper system.

MM 20.15 Tue 14:45 P4

3D Polycrystalline grain structures under the influence of elastic forces — Mathias Reichardt, •Marcus Jainta, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Germany

To predict the failure and strength properties of metallic alloys, it is neccessary to take in account the behaviour of such material under the influence of elastic forces. When applying a sufficient amount of stress, the grain structure breaks and forms a crack. In numerical simulations, we investigate crack propagation in polycrystalline metallic alloys for mode I and III. The shape of such cracks depends on the applied loads and on the grain distribution of the observed material. Suitable simulations require many grains in a relatively large domain. To achieve this goal, we present a parallel, optimized multi phase field model featuring efficient modelling of large three dimensional phase systems coupled with a model for elastic stresses. We show results for 2D and 3D crack developments along grain boundaries and in polycrystalline systems.

MM 20.16 Tue 14:45 P4

From DFT to TB: A reliable derivation of tight-binding parameters for hard materials — •Martin Reese[1,2], Matous Mrovec[1,2], Bernd Meyer[3], and Christian Elsässer[2] — [1]IZBS, Universität Karlsruhe — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [3]ICMM, Universität Erlangen-Nürnberg

Hard materials play an important role in industrial applications as protective coatings of tools. Recent experiments indicate that nanostructered composites of crystalline and amorphous carbides and nitrides can yield materials that reach the limit of super-hardness. However, a scientific understanding of these complex materials is still incomplete.

In the course of developing a multi-scale modelling framework for simulations of nanocrystalline transition metal carbides and nitrides we apply accurate first-principles calculations, based on the density functional theory (DFT), to derive reliable non-orthogonal and orthogonal tight-binding (TB) Hamiltonians. The TB Hamiltonians are constructed by projecting the self-consistent electronic wave functions from DFT onto a minimum basis set of atomic orbitals. This well defined procedure enables to overcome the ad-hoc fitting of TB models and presents a rigorous coarse-graining tool, which can be applied in various bonding environments. In this contribution we will present the application of the method to several model materials, namely the covalently bonded elements carbon and silicon, the transition metal titanium, and binary compounds of these elements. We will discuss the variation of the Hamiltonian matrix elements as a function of the interatomic distance and their transferability in various environments.

MM 20.17 Tue 14:45 P4

Modelling particulate self-healing materials and application to uni-axial compression — •Olaf Herbst[1,2], Akke Suiker[1], and Stefan Luding[2] — [1]Aerospace Engineering, TU Delft, Kluyverweg 1, 2629 HS Delft, The Netherlands — [2]2Multi Scale Mechanics, TS, CTW, UTwente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Using an advanced history dependent contact model for DEM simulations, including elasto-plasticity, viscosity, adhesion, and friction, pressure-sintered tablets are formed from primary particles. These tablets are subjected to uni-axial compression until and beyond failure displaying peak strength. For fast and slow deformation we observe ductile-like and brittle softening, respectively.

We propose a model for local self-healing that allows damage to heal during the loading process such that the material strength of the sample increases and failure/softening is delayed to larger strain. Local healing is achieved by increasing the (attractive) contact adhesion forces for those particles involved in a potentially breaking contact.

We examine the dependence of the strength of the material on (a) the damage detection sensitivity, (b) the damage detection rate, and (c) the (increased) adhesion between healed contacts. The material strength is enhanced, i.e. the material fails at larger strains and reaches larger maximal stress values, when any of the parameters (a) – (c) is increased.

MM 20.18 Tue 14:45 P4

The relationship between the sinter-atmosphere and the phase modification of TiO_2 at high temperatures — •Nicole Pfeiffer, Abdelilah Lahmar, Salah Habouti, Matthias Dietze, Claus-Henning Solterbeck, and Mohammed Es-Souni — Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany

In this work we generated TiO_2-nano particles on Si-substrate by solution deposition from a precursor. The films were treated under different atmospheres at $\sim$800°C to control the phase formation. It is shown by means of Raman scattering that anatase polymorph forms preferentially in reducing atmosphere, instead of the thermodynamically stable rutile phase. The results are discussed in terms of specific defect structures that could form in the anatase phase.

MM 20.19 Tue 14:45 P4

Performance analysis of a parallel simulator for phase-field models — •Alexander Vondrous, Michael Selzer, Britta Nestler, and Marcus Jainta — Institute of Computational Engineering (ICE), Karlsruhe, Germany

Parallel algorithms for the numerical solution of phase field models are used to improve calculation times. To simulate a large section of a complex microstructure and to consider effects such as fluid flow on the morphology evolution, large computational domains have to be considered. In such cases parallelization is needed to significantly increase the speed of the computation. To classify the performance of parallel computations, infomation about the used hardware is important. Performance characteristics are, among others, the speedup and the efficiency. The results of the presented performance analysis are used to optimize parallel algorithms and hardware utilization. The numerical scheme avoids calculations in bulk phase regions of the domain leading to an inhomogeneous load balance and an undesirable higher idle time of some of the CPUs in the network. To minimize this effect, dynamic domain decomposition during run time is applied. Simulations of dendritic growth in a flow field serve to evaluate the performance for different numbers of CPUs.

MM 20.20 Tue 14:45 P4

Polarization dependent Raman spectroscopy of $LiBH_4$ single crystals — •Britta Willenberg, Florian Gebert, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, 38106 Braunschweig, Germany

In a previous paper [1] we have reported an extensive low temperature Raman scattering study on $LiBH_4$ and $LiBD_4$ powders. The 27 observed lines have been assigned to phonon modes within the orthorhombic Pnma structure by comparing the experimental values to density functional theory (DFT) values [1]. In the present contribution we present for the first time Raman scattering measurements on small $LiBH_4$ single crystals. These have been identified among the grains of the powders (Alpha Aesar) by searching for large polarization dependencies of the Raman lines. On the basis of these new results a few of the former assignments have to be revised. Among the external modes this concerns the mode near 307 cm^{-1} which is definitely of A_g symmetry and not of B_{2g} symmetry as had been concluded on purely energy arguments.

A second issue is the phase transition to a hexagonal structure at about 380 K. Several grains of our powder samples did not show the anticipated changes of the Raman spectra. We have now succeeded in finding a few grains which, indeed, display the characteristic simplification of the Raman spectra when the phase transition to the hexagonal phase occurs.

[1] A.-M. Racu et al., J. Phys. Chem. A 112, 9716 (2008)

MM 20.21 Tue 14:45 P4

Low temperature Raman spectroscopy of $Mg(BH_4)_2$ and $Mg(BD_4)_2$ — •Florian Gebert[1], Britta Willenberg[1], Joachim Schoenes[1], Michiel van Setten[2], Christoph Frommen[2], and Maximilian Fichtner[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany

We report a micro-Raman scattering study on fine powders of $Mg(BH_4)_2$ and $Mg(BD_4)_2$ for temperatures ranging from approximately 5K to room temperature. At the lowest temperature, we observe 25 lines in both compounds, which were assigned within the 86 Raman active modes, for the I-4m2 structure, whose energies have been derived using first principle calculations based on density functional theory. This structure was claimed by Ozolins et al. [1] to posses an even lower ground state energy than the $P6_1$ structure reported formerly for the low temperature α-phase [2,3]. The comparison of theoretical and experimental values leads to straight lines with slopes between 0.98 and 1.03 for the external, bending and stretching modes, which is better than expected. Nevertheless, one can not definitively conclude that the structure is I-4m2 since a substantial number of possible lines have not been observed. This is even more so for the $P6_1$ structure. Further progress will require measurements on single crystals and/or intensity computations. [1] V. Ozolins et al., Phys. Rev. Lett. 100, 135501 (2008) [2] R. Cerný et al., Angew. Chem. Int. Ed. 46, 5765 (2007) [3] J.-H. Her et al. , J. Acta Cryst. B63, 561 (2007)

MM 21: Topical Session Nanoporous Functional Materials - Poster

Time: Tuesday 14:45–16:30 Location: P4

MM 21.1 Tue 14:45 P4

Synthesis and Characterization of Nanocomposites for Application as Nanoporous Cathodes in Solid Oxide Fuel Cell — •Azad J. Darbandi[1,2] and Horst Hahn[2,3] — [1]Center for Functional Nanostructures, Universität Karlsruhe (TH) — [2]Gemeinschafts Labor Nanomaterialien, Technische Universität Darmstadt und Forschungszentrum Karlsruhe — [3]Institut für Nanotechnologie, Forschungszentrum Karlsruhe

A recent trend of research on Solid Oxide Fuel Cells is the lowering of the operating temperature for example for Low Temperature Micro-SOFCs. The present work describes the synthesis and a single step coating process of thin film nanocrystalline functional cathode layers. Single phase nanocrystalline (LSCF) cathode powder with ultrafine microstructure and high specific surface area was synthesized via a unique spray pyrolysis process. The powders have been characterized by various methods such as high temperature in-situ X-ray diffraction, DSC-TGA, ICP, HRSEM, TEM, Nitrogen adsorption, Particle size distribution and Zeta-Potential. Yttria stabilized Zirconia substrates were coated with nanodispersion containing LSCF and Gadolinium doped Ceria particles. The electrochemical impedance spectroscopy was carried out on symmetrical samples in dependence of temperature and oxygen partial pressure. The Area Specific Resistance of 50 and 140 mΩ.cm^2 at 700°C and 650°C, respectively, are considerably lower than values reported in literature. High electrochemical activity at low thickness, cost effective coating process and low sintering temperatures are beneficial for low temperature Micro-SOFCs application.

MM 21.2 Tue 14:45 P4

Metals with tunable properties based on porous nanostructures — •Thomas Traussnig[1], Klemens Rumpf[2], Petra Granitzer[2], Stephan Landgraf[3], Heinz Krenn[2], and Roland Würschum[1] — [1]Institut für Materialphysik, Technische Universität Graz, Petersgasse 16, A-8010 Graz, Austria — [2]Institut für Physik, Karl Franzens Universität Graz, Graz, Austria — [3]Institut für Physik. u. Theoret. Chemie, Technische Universität Graz, Graz, Austria

Electric field-induced tuning of material properties is usually restricted to nonmetals such as semiconductors and piezoelectric ceramics. Studies on the property tuning of metals have been initiated recently making use of nanocomposites of porous nanocrystalline metals and liquid electrolytes [1-3]. Owing to the high surface-to-volume ratio of nanoscale metals, voltage-induced formation of electrochemical double layers gives rise to a high fraction of interfacial space-charge regions which results in a reversible change of the overall physical properties of the metal. Studies of the variation of the magnetic behaviour of nanophase metals and alloys upon in-situ charging in a SQUID magnetometer will be presented.

[1] J. Weissmüller et al., Science 300 (2003) 312.
[2] H. Drings et al., Appl. Phys. Lett. 88 (2006) 253103.
[3] M. Sagmeister et al., Phys. Rev. Lett. 96 (2006) 156601

Acknowledgement: Financial support by FWF - Austrian Science Fund (project S10405-N16) is appreciated.

MM 21.3 Tue 14:45 P4

Study on structural and electrical properties of Al-doped ZnO thin films prepared by sol-gel method — •Babak Nasr, Subho Dasgupta, Robert Kruk, and Horst Hahn — Forschungszentrum Karlsruhe, Institute for Nanotechnology, D-76344 Eggenstein-Leopoldshafen, Germany

The screening length of the external field is one of the critical parameters to tune the transport properties of a material. Therefore, the systems of interest are those with carrier concentrations in the same order as the induced maximum surface charge density achievable. In view of this criterion we choose Al-doped ZnO (AZO) oxides with a near metallic conductivity, and a carrier density easily controllable via Al doping. This study is an attempt to optimize conductivity of the nanocrystalline films through the Al concentration and morphology modifications.

The AZO thin films were prepared by the sol-gel process [1]. The thin film deposition was carried out by spin-coating technique on high quality float glass substrates. The film structure and morphology were characterized by profilometer, X-ray diffraction, Scanning Electron Microscopy and Transmission Electron Microscopy. The transport properties were measured with the four point resistance and Hall-effect measurements using standard van der Pauw geometry. The effects of precursor concentrations, annealing temperature on the structural and electrical properties are discussed.

[1] S. Y Chang, Y. Hsiao, Y. Huang, Surface and Coatings Technology, 202 (2008) 5416

MM 21.4 Tue 14:45 P4

Nanoindentation and micro-compression testing of nanoporous gold — •Eike Epler[1], T. John Balk[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen — [2]Department of Chemical and Materials Engineering, University of Kentucky

Recent studies on materials such as nanoporous Au have shown that the strength of open-cell foams can be increased at a fixed porosity by decreasing the foam length scale (ligament diameter and length). This effect is attributed to the difficulty of activating dislocations in sub-micron crystal volumes. If high strength nanoporous materials are to be used to advantage in technical applications, the details of the parameters determining their strength need to be understood.

In this study, the mechanical response of nanoporous Au fabricated by electrochemical dissolution from a Au-Ag alloy, is investigated by indentation using a cube corner tip as well as by micro-compression testing of columns fabricated by focused ion beam machining. The tests reveal a significant time-dependence or creep behavior in the 30% relative density foam that is not observed in fully dense gold. The origins of this effect will be probed by varying the length scale of the foam. In addition, a large scatter in mechanical behavior, particularly in the elastic response, is observed from position to position and sample to sample, which is attributed to small variations in the open cell structure.

MM 21.5 Tue 14:45 P4

Thermodynamic Investigations of Nitrogen confined in Mesopores — •Sebastian Mörz and Patrick Huber — Technische Physik, Universität des Saarlandes, Saarbrücken

The thermodynamic behaviour of nitrogen confined in a mesoporous silica matrix (SBA-15) has been studied by differential scanning calorimetry (DSC) in the temperature range from the bulk melting point down to 42 K and as a function of the filling fraction of the matrix. The heat capacity shows a single melting anomaly in the vicinity of 55 K and a complex freezing anomaly between 47 K and 52 K

Additionally, the structure of the confining matrix has been studied by sorption isotherms which reveal a pore size distribution consisting of uniform mesopores as well as a pronounced corona of micro- and smaller mesopores.

MM 21.6 Tue 14:45 P4

Phase Transitions and Molecular Dynamics of n-Alcohols Confined in Mesoporous Silicon — •Rene Berwanger and Rolf Pelster — Universität des Saarlandes, Saarbrücken, Germany

We have studied phase transitions and molecular dynamics of several n-alcohols in their bulk state and confined into nanotubes with a diameter of 8 nm (mesoporous silica). For this purpose we have combined x-ray, infrared and dielectric measurements. Under confinement the transition temperatures are lowered by up to approximately 30 K. In addition, there is a fundamental structural difference in the crystalline phase. While the bulk alcohols exhibits a polycrystalline mixture of orthorhombic β- and monoclinic γ-forms, geometrical confinement favors the more simple β-form: only crystallites are formed, where the chain axis are parallel to the layer normal. However, the γ-form, in which the chain axis are tilted with respect to the layer normal, is suppressed. A reason for this might be the irregular shape of the nanotubes, into which the crystallites have to fit, favoring the formation of the geometrically more simple and less bulky form. The β-crystallites form bi-layers, that are not randomly orientated in the pores. The molecules are arranged with their long axis perpendicular to the pore axis and parallel to the plane normal of the respective silicon facets (the [011] and [0-11] direction of the silicon matrix).

MM 21.7 Tue 14:45 P4

Dynamics and Structure of n-Nonanol Confined in Silicon

Nanochannels — •Christoph Schuhmacher, Rene Berwanger, and Rolf Pelster — Universität des Saarlandes, Saarbrücken, Germany

The behavior of the short n-alcohol $C_9H_{19}OH$ as bulk material and confined in tubular meso-pores of porous silicon has been studied by infrared spectroscopy. The porous silcicon samples were prepared by electrochemical etching and the mean pore-radius was varied from $r = 3$ nm to $r = 15$ nm. Therefore, we are able to study the influence of geometrical confinement on the liquid-crystalline phase transition. We use several vibrations to determine the transition temperatures, for exemple the OH-stretching vibration, the CH_2 scissor vibration or the vibration of the C-C-backbone. We also discuss differences in the crystalline structure of bulk and confined $C_9H_{19}OH$.

MM 21.8 Tue 14:45 P4

Optical birefringence study of molecular ordering in tubular silica nanochannels — •Matthias Wolff[1], Andriy Kityk[2], Klaus Knorr[1], and Patrick Huber[1] — [1]Technische Physik, Universität des Saarlandes, Germany — [2]Institute for Computer Science, Czestochowa University of Technology, Poland

The condensation of different liquids in nanoporous silicon oxide is studied by combined volumetric adsorption isotherm and optical birefringence measurements. Obtained results suggest that molecules adsorbed in the nanoporous matrix exhibit a weak orientational order in the first adsorbed layers. We could also observe continuous paranematic-to-nematic ordering transitions of liquid crystals in the tubular silica nanochannels[1].

(1) A.V. Kityk, M. Wolff, K. Knorr, D. Morineau, R. Lefort, P. Huber: PRL 101, 187801 (2008).

MM 21.9 Tue 14:45 P4

Transfer of length scales and periodicity of nanowires grown in templates — •Hong-Dan Yan[1,2], Peter Lemmens[1,2], Hanno Dierke[1], Andreas Kruse[1], Dirk Menzel[1], Frank Ludwig[3], and Meinhard Schilling[2,3] — [1]IPKM, TU Braunschweig, Germany — [2]IGSM, TU Braunschweig, Germany — [3]EMG, TU Braunschweig, Germany

A series of magnetic and optical metamaterials based on Fe, Ni, Fe_xNi_{1-x} and Au wires in porous alumina templates have been synthesized using electrochemistry. Electron microscopy shows a single wire microstructure with uniform size, a diameter of about 30nm - 90nm, and a length controllable by the deposition time. Magnetic measurements (SQUID) show a hysteresis of the magnetization and an anisotropy switching with wire diameter. Work supported by IGSM.

MM 22: Topical Session Nanoanalytics using Small-Angle Scattering - Poster

Time: Tuesday 14:45–16:30 Location: P4

MM 22.1 Tue 14:45 P4

The ratio of magnetic and nuclear small-angle neutron scattering in neutron-irradiated binary iron alloys — •Frank Bergner and Andreas Ulbricht — Forschungszentrum Dresden-Rossendorf

The effect of neutron irradiation on the formation of defect-solute clusters in binary iron alloys is important for the understanding of the damage mechanisms in structural materials applied in the fields of nuclear technology. These nanoscale features operate as scatterers. The composition of the clusters in terms of solute atoms, iron atoms and vacancies is subject to debate. The A-ratio defined as the ratio of the scattering cross sections perpendicular and parallel to a saturation magnetic field in a sample of a ferromagnetic material provides a link between measurable quantities and cluster composition.

SANS measurements performed for neutron-irradiated binary Fe-Cu, Fe-Ni and Fe-Cr alloys are reported. The analysis is based on the assumption of a two-phase matrix-inclusion topology with inclusions (clusters) fully coherent with the matrix, i.e. clusters consist of atoms of the alloying element, Fe-atoms and/or vacancies confined to lattice sites of a rigid bcc lattice. The values of the A-ratio obtained for Fe-Cu and Fe-Ni can be explained as clusters containing vacancies. The derived vacancy fractions will be specified. For the investigated Fe-9at%Cr alloy the situation is more complex and will be discussed in the paper.

MM 22.2 Tue 14:45 P4

Extending the possibilities of a Kratky-Compact-Camera by use of focussing multilayer X-ray optics — Thomas Henze, •Albrecht Petzold, Klaus Schröter, and Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

The use of focussing multilayer x-ray optics on laboratory x-ray equipment offers the potential of a substantial gain in primary beam intensity without a significant loss of resolution. We present the result of a refurbishment of Kratky-Compact-Camera, a classical setup for small angle x-ray scattering on isotropic samples, with an elliptically bent focussing multilayer. The advantages of the Kratky collimation system are ease of alignment, high intensity and low background. A further gain in intensity is highly desirable for time dependent experiments as well as for measurement of weakly scattering samples. The performance of the revised setup is analyzed quantitatively by comparing intensity and full width at half maximum of the primary beam, as well as the minimal accessible scattering vector with the corresponding parameters of the simple setup without optics. A gain in intensity of a factor 2 up to 10 is achieved, depending on the details of the alignment. In addition the multilayer produces a monochromatic beam. First measurements on expemplary polymer systems are shown.

MM 23: Topical Session Heterogeneous Nucleation and Initial Evolution of Microstructure - Poster

Time: Tuesday 14:45–16:30 Location: P4

MM 23.1 Tue 14:45 P4

Scale-bridging phase-field simulations of microstructure responses on nucleation in metals and colloids — •Denis Danilov and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Germany

Phase-field simulations from atomic to mesoscopic length scales are used to analyse the microstructure responses on heterogeneous nucleation, both in metallic as well as in colloidal systems. The scale-bridging from 1 nm to 10 μm in metals is achieved either by combining Molecular Dynamics (MD) and Phase-field (PF) simulations or by hybrid PF modelling. Essential for three dimensional numerical computations is the employment of performance optimized simulation techniques and adaptive multigrid methods. The microstructure responses on the parameter sets, on the shape of the nuclei and on the characteristic properties of the substrate are systematically investigated in PF simulations. Large-scale simulations of microstructure formations are compared with experimental observations.

MM 23.2 Tue 14:45 P4

Colloidal model system for undercooled metals — •Ina Klassen[1], Patrick Wette[1], Dirk Holland-Moritz[1], Thomas Palberg[2], Stephan V. Roth[3], and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, — [2]Institut für Physik, Johannes-Gutenberg-Universität Mainz, — [3]HASYLAB, DESY, 22603 Hamburg, Germany

Model systems are often used to describe equilibrium properties of simple fluids and solid materials. Charged colloidal spheres in aqueous dispersion show a rich phase behavior and many phenomena known from

metals are also observed here, like selection of the metastable phase at large undercoolings. By contrast to metals heterogeneous nucleation can either be efficiently suppressed or, if present, clearly discriminated and separated from data evaluation. Our colloidal particles are characterized by convenient time scales (seconds) and particle distances (300-500nm) and thus accessible by optical techniques. Microscopy and light scattering yield complementary information on equilibrium properties and crystallization kinetics from real and reciprocal space (phase behavior, solidification mechanisms, growth velocities, nucleation rate densities). Structural changes of the melt with increased undercooling and the corresponding changes of the solidification can be monitored by Ultra Small Angle X-Ray Scattering (USAXS) performed at HASYLAB (Hamburg).

MM 23.3 Tue 14:45 P4

Heterogeneous nucleation in charged colloidal model systems using spherical seeds: Controlling the crystallization kinetics — •Andreas Engelbrecht, Roushdey Salh, Thomas Palberg, and Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

In the classical crystallization scenario three processes can be discriminated: crystal nucleation, growth and ripening. The crystallization kinetics and the resulting morphology of the polycrystalline material are given by a complex interplay of these mechanisms. Controlling nucleation and growth is one key to create new materials. A great deal of progress has been made in recent years using colloidal suspensions as model systems studying crystallization. Close analogies to atomic systems are observed which can be exploited to address questions not accessible in atomic solidification. We here present systematic measurements controlling the crystallization kinetics of a charged colloidal model system by adding small amounts of a second higher charged component. Using small amounts of the second component the nucleation rate is strongly accelerated whereas crystal growth is only slightly influenced. At large amounts the crystallization process is overshadowed by fractionation of the supersaturated fluid: nucleation is delayed and crystal growth slowed down. The average crystal size of the resulting polycrystalline material can be changed by a at least one order of magnitude. The crystal size distribution is strongly influenced in its shape as well.

MM 23.4 Tue 14:45 P4

Surface Tension of Liquid Al-Cu Alloys — •Julianna Schmitz, Jürgen Brillo, and Ivan Egry — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Precise surface tension data of liquid Al-Cu alloys are fundamental for our purpose of studying the interaction of the liquid with differently oriented single crystalline sapphire surfaces. These data were measured for the entire Al-Cu liquid alloy system as a function of temperature and composition. Contamination of the sample from contact with container walls had to be avoided. Thus, measurements were performed in an inert gas atmosphere using an electromagnetic levitation furnace. From surface oscillations of the levitated droplet the surface tension was determined by means of the oscillating drop method. Hence, we obtained precise data of the entire Al-Cu system within a wide temperature range with only a small scatter of 3%. A linear temperature dependence with a negative slope was found for all stoichiometric compositions whereas the surface tension monotonically decreases with increasing aluminium concentration. The observed behaviour with respect to both, temperature and concentration, is in agreement with thermodynamic model calculations using the regular solution approximation. Additionally, we give an outlook on the measurement of contact angles and the work of adhesion as a function of the crystalline substrate orientation performed with a sessile drop apparatus whose construction is about to be finished. Combining this with the surface tension data we are able to estimate solid-liquid interfacial energies.

MM 23.5 Tue 14:45 P4

Heterogeneous nucleation undercooling and kinetics analysis — •Charuayporn Santhaweesuk[1], John H. Perepezko[1], Joachim Bokeloh[2], and Gerhard Wilde[2] — [1]University of Wisconsin-Madison, Department of Materials Science and Engineering, Madison, USA — [2]University of Münster, Institute of Materials Physics, 48149 Münster, Germany

For large liquid volumes it is essential to remove or to deactivate heterogeneous nucleation sites in order to achieve large undercooling values. An effective method of melt conditioning for nucleant removal is based upon flux treatments, but the mechanism that is responsible for the large undercooling is not properly understood. Recent experiments and analyses of the undercooling behavior in flux treated pure Cu have provided new results as well as confirmation for a model of nucleant refining that accounts for the undercooling behavior including initial conditioning, atmosphere effects and saturation in a self-consistent manner. Moreover, the statistical analysis of the undercooling data that has been developed during the initial work on pure Au can yield nucleation rates that are independent of the choice of a specific nucleation kinetics model. These results are also discussed in comparison with a description based on classical nucleation theory.

MM 23.6 Tue 14:45 P4

Binary Mixtures of Charged Colloidal Suspensions and their Role as Model Systems — •Nina J. Lorenz[1], Patrick Wette[2], Thomas Palberg[1], Hans Joachim Schoepe[1], and Tsuneo Okubo[3] — [1]Institute of Physics, University Mainz, Germany — [2]Institute for Raumsimulation DLR Cologne, Germany — [3]Cooperative Research Centre, Yamagata University, Yonezawa, Japan,

We investigate colloidal charged sphere mixtures in aqueous dispersion, exploring their possible use as conveniently accessible models for metallic binary mixtures. Using static and dynamic light scattering, torsional resonance spectroscopy and optical microscopy we investigate the structure, elasticity and solidification kinetics of mixtures with different size- and charge ratio. We find a rich variety of binary phase diagrams similar to those in metal systems including spindle, azeotropic and eutectic types [1, 2]. Eutectic-like behaviour is found for large asymmetries in the mixtures and demixing confirmed by diffusion experiments. The independent solidification of the segregating components is monitored with time resolved elasticity measurements. In addition we find interesting morphologies not unlike those in metal eutectics, but still considerably altered due to the different system dynamics. [1] T. Palberg, N. Lorenz, H.J. Schoepe, P. Wette, I. Klassen, D. Holland-Moritz, D.M. Herlach, in D. Herlach et. al.: Solidification in multicomponent melts, VCH-Wiley Weinheim, 2008, pp. 185-212, Solidification experiments in single component and binary colloidal melts [2] N. Lorenz, J.Liu, T. Palberg: Phase behaviour of binary mixtures of colloidal charged spheres, Colloids Surf. A 319, 109 (2008)

MM 23.7 Tue 14:45 P4

Numerical Simulation of Heterogeneous Nucleation and Microstructure Formation in Al-Ni Alloy System — •Ricardo Siquieri[1], Evelyn Doernberg[2], Heike Emmerich[1], and Rainer Schmid-Fetzer[2] — [1]Computational Materials Engineering, Center of Computational Engineering Science and Institute of Minerals Engineering, RWTH Aachen, Mauerstrasse 5, D-52064 Aachen, Germany — [2]Institut für Metallurgie, Robert-Koch-Straße 42, 38678 Clausthal-Zellerfeld, Germany

Many important technological materials including magnetic and superconducting alloys are produced through solidification in peritectic systems. Although this class of materials is very important for the industry, many aspects of its solidification process are still unclear. To help with gaining a comprehensive and reliable understanding of this process, we will present numerical investigation of peritectic solidification for the system Al-Ni alloy in this contribution. For this purpose, recent developments of phase-field field techniques will be combined with thermodynamic precision data aiming a systematic investigation of all stages of peritectic solidification: Heterogeneous nucleation, peritectic reaction, peritectic transformation, and direct growth of the peritectic phase. This model approach allows us to make conclusions based on its comparison with experimental measurements as well as employ it to obtain new relations between processing parameters and the resulting kinetics and dynamics of the phase-transformation process during all of the four stages above.

MM 23.8 Tue 14:45 P4

Elastic effects on heterogeneous nucleation and microstructure formation — •Robert Spatschek[1], Efim Brener[2], Michael Fleck[2], Clemens Gugenberger[2], Claas Hüter[2], Heiner Müller-Krumbhaar[2], Denis Pilipenko[2], and Alain Karma[3] — [1]ICAMS, Ruhr-Universität Bochum — [2]IFF-3, Forschungszentrum Jülich — [3]Northeastern University Boston

Elastic effects due to lattice strain modify the local equilibrium conditions at solid-solid interfaces compared to classical dendritic growth. We present results on the influence of dilatational and shear strain on the kinetics of these phase transitions and discuss its relevance for the selection properties.

The description of surface-diffusion controlled dynamics via the phase-field method is less trivial than it appears at first sight. Numerical simulations of a standard and a more sophisticated model from the literature as well as of two new models are performed to assess the relative merits of each approach.

On small scales, the overlap of interface profiles can lead to attractive and repulsive forces, which are important for the understanding of heterogeneous nucleation processes. They are related to lattice incompatibilities due to a misorientation or grain shifts, and provoke elastic deformations and the formation of dislocations. Using concepts from the classical density functional theory and amplitude equations we shed light on the forces between solid-melt interfaces on an analytical and numerical level.

MM 23.9 Tue 14:45 P4

Derivation of the phase field crystal model for colloidal solidification — •Sven van Teeffelen[1], Rainer Backofen[2], Axel Voigt[2], and Hartmut Löwen[1] — [1]Institute for Theoretical Physics II: Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf — [2]Institute of Scientific Computing, Technical University Dresden, D-01062 Dresden, Germany

The phase-field crystal model is by now widely used in order to predict crystal nucleation and growth. For colloidal solidification with completely overdamped individual particle motion, we show that the phase-field crystal dynamics can be derived from the microscopic Smoluchowski equation via dynamical density functional theory. The different underlying approximations are discussed. In particular, a variant of the phase-field crystal model is proposed which involves less approximations than the standard phase field crystal model. We finally test the validity of these phase-field crystal models against dynamical density functional theory. In particular, the velocities of a linear crystal front from the undercooled melt are compared as a function of the undercooling for a two-dimensional colloidal suspension of parallel dipoles. Good agreement is only obtained by a drastic scaling of the free energies in the phase field crystal model in order to match the bulk freezing transition point.

MM 23.10 Tue 14:45 P4

Computer simulation studies of heterogeneous nucleation in the hard spheres and colloid-polymer mixtures. — •Tatyana Zykova-Timan[1], Juergen Horbach[2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Using Monte Carlo simulations in $NP(z)T$ ensemble a growth of the crystalline germ on the planar walls is modeled. Both hard spheres and colloid-polymer mixtures were considered. The latter was represented by one-component colloid system described by an effective Asakura-Oosawa potential. The repulsive interactions between the wall and colloids were tuned such that no wetting layer was allowed. We show how to stabilize the solid nucleus on the wall and analyze its morphology.

MM 23.11 Tue 14:45 P4

Phase field modeling vs. molecular dynamics simulations: Crystal growth kinetics of Ni — •Roberto Rozas Cardenas[1], Denis Danilov[2], Britta Nestler[2], and Jürgen Horbach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — [2]Institute of Computational Engineering (ICE), Karlsruhe University of Applied Sciences, Moltkestrasse 30, 76133 Karlsruhe

Growth of crystal seeds in the undercooled melt of pure Nickel is simulated by means of molecular dynamics simulations and phase-field modeling. In order to establish a direct comparison between the two methods the lower length-scale limit of the phase field modeling is extended up to the scale of typical molecular simulations, i.e. about 100 Å. The input variables of the phase field modeling such as interface tension and transport properties, and initial configurations, are obtained from molecular dynamics simulations. We present results for the growth velocities of crystal seeds of Ni at different undercoolings. The validity of the assumptions of the phase modeling at nanoscopic scale is discussed.

MM 24: HV Hassel

Time: Wednesday 9:30–10:00 Location: IFW A

Invited Talk MM 24.1 Wed 9:30 IFW A

From eutectic alloys to metal nanowires — •Achim Walter Hassel — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Solidification of eutectic alloys is an invariant reaction in which both phases solidify simultaneously without changing the composition of the melt. Directional solidification of a eutectic alloy of asymmetric composition for example in a Bridgman furnace produces iso-oriented single crystalline metal nanowires embedded in a single crystalline matrix. Electrochemically a highly selective and precisely controllable release is possible. W, Mo, Re and Cu wires can be produced as well as Au nanobelts. A thorough characterization by HRSEM, TEM, EBSD, AFM, XRD, XPS, GDOES and ICP-OES yields a comprehensive view of these objects. Examples will illustrate that a number of interesting applications are possible such as STM tips, pH-sensors, catalysts, NEMS resonators and model samples for mechanical studies. An outlook will indicate further developments in this field.

MM 25: Topical Session High Temperature Materials I

Time: Wednesday 10:15–12:15 Location: IFW A

Topical Talk MM 25.1 Wed 10:15 IFW A

Intermetallic phases for structural applications at high temperatures — •Martin Palm — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany

Intermetallic phases - intermetallics for short - have evolved within the last 25 years from being only of interest to scientists because of their sometimes peculiar crystallographic structures and fascinating physical properties, to form the basis for a new class of materials that have proven their capability to be used for structural applications up to very high temperatures and in demanding environments. In general intermetallics often have relatively high melting temperatures, sometimes above those of the constituting elements, and in addition they may offer other attractive properties such as an outstanding corrosion resistance, remarkable low density and superior mechanical properties. Therefore, a considerable number of material developments have taken place in order to exploit their potential for structural applications at high temperatures. In the focus of these developments were the aluminides, namely Ni3Al, NiAl, Ti3Al, TiAl, Fe3Al and FeAl, though also silicides and some more specific intermetallics have gained attention. The presentation will give an overview about properties which make intermetallics that attractive for high temperature applications, a summary on individual material developments such as gamma titanium aluminides as well as addressing current research issues.

Topical Talk MM 25.2 Wed 10:45 IFW A

Deformation Behavior of Mo-Si-B Alloys — •Sharvan Kumar — Division of Engineering, Brown University, Providence, RI 02912, USA

Mo-rich Mo-Si-B alloys are being considered as possible candidates for ultra-high-temperature applications and therefore properties of interest include strength and ductility, toughness and fatigue response of both, the multiphase alloys as well as the Mo solid solution phase. In

this presentation, the tensile and compressive creep response of two- and three-phase alloys, crack growth behavior during monotonic and cyclic loading, as well as the contribution of creep in adversely affecting fatigue response will be discussed. These studies helped identify regimes where the microstructure ahead of the crack tip revealed several instabilities including recrystallization, grain growth and creep cavitation. Further, it became apparent from these studies that the Mo(Si,B) solid solution plays a dominant role in influencing toughness and creep resistance, and therefore mandated detailed examination in isolation. Tensile studies on the single phase Mo-Si-B solid solution phase has confirmed dynamic strain aging (DSA), and comparative studies on pure Mo (containing comparable levels of O and C) point to the important role of B and Si in solution on DSA in the solid solution alloy. The presentation will close with a brief discussion on the more recent advances in this alloy system and the challenges, barriers and potential for further development.

MM 25.3 Wed 11:15 IFW A

Herstellung und Charakterisierung von einkristallinen lamellaren und faserverstärkten Werkstoffen in den Systemen Cr-Cr_3Si und NiAl-Mo(Cr) — •Titus Haenschke[1], Martin Heilmaier[2], Easo George[3] und Manja Krüger[1] — [1]Otto-von-Guericke-Universität, Institut für Werkstoff- und Fügetechnik, 39104 Magdeburg, Deutschland — [2]TU Darmstadt, Physikalische Metallkunde, 64287 Darmstadt, Deutschland — [3]Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN 37831-6093, USA

Gerichtet erstarrte Legierungen in den eutektischen Systemen NiAl-9Mo, NiAl-34Cr und Cr-Cr_3Si sind vielversprechende Kandidaten, um Nickelbasis-Superlegierungen in konstruktiven Hochtemperaturanwendungen zu ersetzen. Im Rahmen dieser Arbeit wurden NiAl-X-Kristalle mit Wachstumsgeschwindigkeiten von 20 und 80 mm/h und Cr-Cr_3Si-Kristalle mit 60, 120 und 160 mm/h gezüchtet. REM-Analysen des Gefüges zeigten bei den NiAl-X-Systemen in Schnitten senkrecht zur Kristallwachstumsrichtung eine faserverstärkte gleichmäßige Struktur. EBSD-Analysen zeigten jedoch, dass nicht immer wie erwartet Einkristalle hergestellt werden konnten. Bei den Cr-Cr_3Si-Kristallen liegt eine gut ausgebildete lamellare Struktur vor. Die Durchführung von Drei-Punkt-Biege- und Druckversuchen bei verschiedenen Temperaturen diente zur Ermittlung mechanischer Kennwerte und der Spröd-Duktil-Übergangstemperatur. An gebrochenen Biegeproben fanden REM-Untersuchungen der Bruchfläche statt. Erste Druckversuche unter konstanter Spannung dienen der Abschätzung des zu erwartenden Kriechwiderstandes der untersuchten Werkstoffe.

MM 25.4 Wed 11:30 IFW A

Structure, Chemical Stability and Properties of NiAl-Al2O3 Interface Modified by hBN and MAX-Phase Interlayers — •Jia Song, Weiping Hu, Yunlong Zhong, Hao Chen, and Günter Gottstein — Institut für Metallkunde und Metallphysik, Kopernikus Strasse 14, 52056 Aachen, Germany

The interlayers from different materials were used in order to modify the interface structure/property and to improve the mechanical properties of NiAl composites reinforced by continuous single crystal Al2O3 fibers. It was found that the interface without interlayer had a good chemical stability during hot pressing (sample fabricating), resulting in high interface shear strength (about 250 MPa) at RT. But for the composites with interlayers, chemical reactions occurred in the interfacial area during diffusion bonding. In the interfacial area with a hBN interlayer the chemical reaction between BN and NiAl led to the formation of an AlN sublayer and precipitation of nanocrystalline NiAl particles in hBN. The interface shear strength is about 70 MPa. For composites with the V2AlC interlayer, chemical reactions resulted in a complete decomposition of interlayer and formation of varied reaction products. The corresponding interface strength is about 32 MPa. For the case of Cr2AlC interlayer, it was transformed into two sublayers: C-rich sublayer on the fiber side and Cr-rich sublayer next to the matrix. Fine Al2O3 and carbon particles were precipitated in the Cr-rich sublayer and in the Al2O3 fiber respectively. The interfacial shear strength is about 110 MPa. The possible influences by introducing the interlayers on mechanical performance of NiAl composites are discussed.

MM 25.5 Wed 11:45 IFW A

High Temperature Stability of Nanostructured Amorphous Si-C-N Materials — Wolfgang Gruber and •Harald Schmidt — TU Clausthal, Institut für Metallurgie, AG Materialphysik, Germany

Polymer-derived Si-C-N ceramics are a new class of multifunctional high temperature materials with applications in various branches of technology. After synthesis, these materials consist of amorphous nanodomains which are expected to have a crucial importance for the extraordinary high temperature stability. Annealing at temperatures above 1400 °C leads to formation of nanocrystalline precipitations. We investigated the thermal stability, nanodomain growth and crystallization behaviour of these ceramics using XRD and small angle scattering techniques as well as diffusion studies. A model based on diffusion controlled nanodomain growth is proposed to explain the high temperature stability.

MM 25.6 Wed 12:00 IFW A

Microstructure and properties of Co-Re-based experimental alloys for high temperature applications — •Debashis Mukherji[1], Joachim Rösler[1], Rainer Hüttner[2], Uwe Glatzel[2], Timo Depka[3], Christoph Somsen[3], Gunther Eggeler[3], Manja Krüger[4], and Martin Heilmaier[4,5] — [1]Technische Universität Braunschweig, Braunschweig, Germany — [2]Universität Bayreuth, Bayreuth, Germany — [3]Ruhr-Universität Bochum, Bochum, Germany — [4]Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany — [5]Technische Universität Darmstadt, Darmstadt, Germany

New high temperature materials are needed to substitute Ni-base superalloys above 1200°C. Co-Re based alloys are being developed at TU Braunschweig, for this purpose. Re (high melting) forms a continuous solid solution with Co and increases melting point of Co-alloys. Various hardening mechanisms is explored in Co-Re-Cr-C system; namely solid solution hardening by Re, precipitation strengthening by carbides and composite strengthening by - hard (Re-rich) and soft (Co-rich) phases. Unlike in the conventional Co-alloys, where the matrix is fcc, in Co-Re alloy the matrix is hcp phase. The morphology and distribution of second phases are important parameters for effective strengthening. For application in gas turbine the long term stability of the microstructure and high temperature mechanical properties are important. Study of microstructure stability and mechanical properties at high temperatures on two experimental alloys Co-17Re-23Cr and Co-17Re-23Cr-2.6C [compositions in at%] will be presented.

MM 26: Nanostructured Materials I

Time: Wednesday 10:15–11:15 Location: IFW B

MM 26.1 Wed 10:15 IFW B

Photoexcitation of Volume Plasmons in Metallic Nanostructures — •Katja Ehrhold[1], Ulrich Gösele[1], and Silke Christiansen[2,1] — [1]Max-Planck-Institut, Weinberg 2, 06120 Halle — [2]Institut für Photonische Technologien, Albert-Einstein-Str. 9, 07745 Jena

It has long been known that a vanishing permittivity enables longitudinal electromagnetic waves. The corresponding collective eigenmodes called volume plasmons should not be dipole excitable in classical electrodynamics. Thus, the typical volume modes are known to be excitable via particle beams solely.

We investigated typical scattering problems for an incident plane wave determined via the Helmholtz-equation which can be solved analytically for special geometries. The analytical solution for a spherical scatterer by Gustav Mie was extended to spherical core-shell structures by Aden. Remarkably, in the case of metallic nanoshell structures the Mie extinction efficiencies have a local maximum at the natural plasma frequency corresponding to the photoexcitation of a volume plasmon. This volume mode is independent of both the shell's aspect ratio and the core material. For explanation we present a simple physical picture which is supported by analytical examples on silver and gold shells. Additionally we use finite element simulations to show a potpourri of particles which likewise enable the photoexcitation of volume modes.

MM 26.2 Wed 10:30 IFW B

Formation of dendritic metallic nanowires — •Nitesh Ranjan[1], Hartmut Vinzelberg[2], and Michael Mertig[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Recently, we reported an electrical-field-controlled growth process for the directed bottom-up assembly of one-dimensional palladium nanowires between micro-fabricated electrodes [1]. The wires, grown from an aqueous palladium salt solution by dielectrophoresis, had a thickness of only 5-10 nm and a length of up to several micrometers. The growth process was found to depend largely on the deposition conditions like the strength and the frequency of the applied AC field and the concentration of the metal salt solution. Here, we report the formation of thin, but straight and dendritic metallic nanowires, obtained in the low-frequency regime. The morphology of the wires was characterized by scanning force microscopy (SFM), scanning electron microscopy and transmission electron microscopy. SFM investigations revealed that the palladium nanowires grown over the glass and silicon substrates have a typical thickness of about 25 nm. Room temperature I-V measurements show them to be Ohmic in nature with a resistance of about 80 kOhm. Low-temperature measurements show the phenomenon of zero bias anomaly. The investigated growth method is capable of controllable in-place formation of complex circuit patterns for future nanoelectronics. [1] Nitesh Ranjan, Hartmut Vinzelberg, Michael Mertig, Small 2, 1490 (2006).

MM 26.3 Wed 10:45 IFW B

A structure-induced metal-insulator transition in thin MoS nanowires — Igor Popov[1], Gotthard Seifert[1], and •Sibylle Gemming[2] — [1]Theoretische Chemie, TU Dresden, D-01062 Dresden, Germany — [2]Forschungszentrum Dresden-Rossendorf, P.O.Box 510119, D-01314 Dresden, Germany

Transition metal chalcohalides MX2 can form a wealth of diverse nanostructures, which range from large octahedral and fullerene-like hollow clusters and cylindrical nanotubes close to the nominal composition M:X = 1:2 to smaller, two-dimensional platelet-shaped clusters under sulfur excess and to one-dimensionally elongated nanowires under sulfur-deficient conditions. All of those structures exhibit specific electronic properties that differ from the ones of the pure bulk and open up a large application spectrum, that includes the lubricant aspect, but extends to catalysis and electronic transport. One-dimensionally delocalized electronic states provide the basis for the higher activity, reactivity and conductivity in such nanostructures. One-dimensional MX wires are composed of a central metallic wire coated by a sulfur and/or halide shell. They exhibit a very high structural regularity, hence, ballistic conductivity may be obtained in such structures. DFT calculations showed that wires can act as electromechanical switches, because they undergo a symmetry-dependent metal-insulator transition upon twisting [Nano Lett.,10.1021/nl801456f; Nano Lett., 2008, 8, 3928-3931].

MM 26.4 Wed 11:00 IFW B

Conductivity and shot noise in graphene at high bias voltages — •Aurelien Fay[1], Romain Danneau[1,2], Fan Wu[1], Matti Tomi[1], Julien Wengler[1], and Pertti Hakonen[1] — [1]Low Temperature Laboratory, Helsinki University of Technology, Espoo, Finland — [2]Institut für Nanotechnology, Forschungszentrum Karlsruhe, and Physikalische Institut, Universität Karlsruhe, Karlsruhe, Germany

The conductivity and the shot-noise in graphene contain both interesting informations on the transport properties of the Dirac fermions. By measuring these two quantities, we have shown that the transport in Graphene could be ballistic [1]. The interaction between optical phonons and charge carriers in graphene can suppress this ballistic transport and, therefore, dramatically changes the conductivity and the Fano factor.

We have increased the electron-phonon coupling in graphene by subjecting the graphene sample at high bias voltages [2]. At a relative low bias, we have measured a linear dependence of the conductivity as a function of the bias voltage. This has been recently pointed out by E. Sonin [3]. In the high bias regime, the decrease of the conductance and the drop of the Fano factor could both be explained by the interaction between optical phonons and charge carriers.

[1] R. Danneau *et al.*, Phys. Rev. Lett. **100**, 196802 (2008).
[2] W.K. Tse *et al*, Appl. Phys. Lett. **93**, 023128 (2008)
[3] E. B. Sonin, Phys. Rev. B **77**, 233408 (2008).

MM 27: Interfaces I

Time: Wednesday 11:30–12:45 Location: IFW B

MM 27.1 Wed 11:30 IFW B

Grain boundary migration by molecular-dynamics simulation — •Jian Zhou, Volker Mohles, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, Aachen

Molecular dynamics simulations have been used to study grain-boundary migration of three series ([001], [011], [111]) of twist grain boundaries (GBs) in copper. An orientation-correlated force being able to drive flat GBs with different misorientations was applied to all twist GBs. The temperature dependence of the GB mobility was determined over a wide misorientation range. It is found that there is an obvious reduction in activation enthalpy with respect to GB migration when the temperature rises to a certain point for many high-angle and high-energy GBs. This reduction could be attributed to the structural change in GBs, such that different GB migration mechanisms become active. Moreover, GB structures were characterized by common neighbor analysis at low temperature. For low-angle GBs, a network of screw dislocations were traced, and it was found that this structure is relatively stable during the GB migration process. For high-angle GBs, in contrast, much more complicated and spatially extended GB structures were observed, which move mainly by a collective shuffle mechanism.

MM 27.2 Wed 11:45 IFW B

Phase-field modelling of foam microstructure evolution — •Frank Wendler, Eduard Stirner, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Moltkestr. 30, 76133 Karlsruhe, Germany

Foam is a cellular materials with large variety of applications ranging from metal or polymer foams to cosmetics. After generation, a foam is a liquid with a complex rheological behaviour, dominated by surface free energy minimisation towards configurations of local equilibrium. We adapt a general multi phase-field model to describe this evolution step, important for the mechanical properties of a solidified foam material. Starting with a volume preserving Allen-Cahn model for incompressible dry foams with negligible liquid fraction (e.g. soap froth), a pressure dependant term is added to the functional of the free energy. This allows for the treatment of bubbles filled with a compressible gas. Assuming homogeneous pressures related to an equation of state a consistent model of boundary evolution can be given. The results approve that pressures within single bubbles are related to interface curvature according to the Young-Laplace equation. Simulations of bubble clusters and foam structures in 2D and 3D are presented, including the examination of pressure variations as a process step to optimize structure and accelerate equilibration. Finally, the treatment of wet foams with a non-negligible fraction of liquid, concentrated along the Plateau borders is given. Numerical evaluation of surface energies and dynamics show that it is not necessary to completely resolve the diffuse interface, which enables the simulation on larger length scales.

MM 27.3 Wed 12:00 IFW B

Simulations of surface energy driven processes at structured substrates — •Marcus Jainta and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

We introduce a new method based on a phase-field model to simulate the behaviour of multiple phase regions at given non-moving obstacles with sharp interfaces in terms of new boundary conditions. We discuss the results for different surface energies of the simulated microstructures and bubbles. In addition, we consider adhesion forces in the presence and absence of fluid flow. The simulation results of liquid droplets on structured surfaces are compared with experiments related to the Lotus effect. Finally we discuss the numerical method and implementation of the new boundary conditions.

MM 27.4 Wed 12:15 IFW B

3D Vertex Dynamics Simulation of Grain Growth in Ceramics Including the Anisotropy of Grain Boundary Energy — •Melanie Syha[1], Ling Yue[1], Daniel Weygand[1], and Peter Gumbsch[1,2] — [1]Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen — [2]Fraunhofer IWM, Freiburg

A three dimensional (3D) vertex dynamics model for grain growth is presented, adapted to the study of grain growth in Strontium-Titanate-Oxide (STO) ceramics. The 3D vertex dynamics model for grain growth is an interface tracking model [1]. In this approach grain boundaries (GB) are discretized and their time evolution is derived from the minimization of the GB energy, which is dissipated by the motion of the GBs and triple lines. The original model [1,2] has been extended to handle misorientation and inclination dependent GB energies, mobilities and triple line drag. The improved model is compared to the 3D analogue of the Neumann-Mullins law [3].

The influence of structure dependent GB properties on statistical observables, e.g. grain size distribution function, grain growth dynamics and correlation function between grain size and number of neighboring grains is investigated. Cross sections through the grain structures are analyzed and compared to experimental observations on grain growth in STO ceramics

[1] D. Weygand, Y. Bréchet, J. Lépinoux, and W. Gust, Phil. Mag. B 79 (1999) 703. [2] D. Weygand, Y. Bréchet and J. Lépinoux, Interface Science 7 (1999) 285. [3] R. MacPherson and D. Srolovitz, Nature 446 (2007) 1053

MM 27.5 Wed 12:30 IFW B

THE FINITE MOBILITY OF THE BOUNDARY JUNCTIONS AND THE THEORETICAL PREDICTIONS OF GROWTH RATE FOR POLYCRYSTALS UNDERGOING GRAIN GROWTH — •Luis Barrales-Mora — Institut für Metallkunde und Metallphysik, RWTH-Aachen, Aachen, Germany

As a consequence of the recent demonstration of the three-dimensional von Neumann-Mullins relationship by MacPherson and Srolovitz, there has been a renewed interest in the investigation of the phenomenon known as grain growth. This interest arises from the many possibilities that this new relationship offers but also, and contradictorily, from its limitations. One of such limitations is the impossibility of this relationship to predict correctly the volume rate of change of grains if the motion of the grain boundaries is hindered. It is well known that many factors can hinder the grain boundary motion, e.g., second-phase particles, impurity atoms, the finite mobility of the boundary junctions, etc. In the present contribution, the latter factor is analysed in light of the Cahn-MacPherson-Srolovitz relationship by means of computer simulations. This relationship is coupled with theories on the finite mobility of triple lines and quadruple junctions and compared with simulation results in single grains. Similar relationships by Glicksman and Rios and Hilgenfeldt et al. are also investigated. This last point is relevant since these approaches allow the study of grain growth from a more statistical point of view.

MM 28: Electronic Properties I

Time: Wednesday 10:15–11:45 Location: IFW D

MM 28.1 Wed 10:15 IFW D

The Tuneable Electron Mobility in Charged Indium Tin Oxide Thin Films — •Subho Dasgupta, Maya Lukas, Robert Kruk, and Horst Hahn — Institute for Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany

This study aims at the quantitative understanding of the change in electronic transport upon surface charging in nanoparticulate and nanocrystalline conducting oxide. Previously, we demonstrated a device with a metallic conducting channel made of Indium Tin Oxide (ITO) nanoparticles which exhibits an on/off ratio of 2×10^3 [1]. To find the mechanism of such a large change in conductivity, we prepared nanocrystalline ITO thin films of a few nanometers thickness as a model system. It was observed that an increase in the Sn-doping level near the grain boundaries results in a local variation in the screening length upon charging. This variation is considered to be equivalent to an increase in the surface roughness resulting in the disruption of the conducting paths. It is concluded that primarily a change in the scattering probability is causing the high value of variation in transport properties for highly-doped semiconductors like ITO.

[1] S. Dasgupta, S. Gottschalk, R. Kruk, H. Hahn, Nanotechnology 19 (2008) 435203

MM 28.2 Wed 10:30 IFW D

The electrical properties of anodically oxidized Ti based NWFETS and its oxygen sensor applications — •Dawit Gedamu, Seid Jebril, Arnim Schuchardt, and Rainer Adelung — Functional Nanomaterials, Institute of Materials Science, Faculty of Engineering, CAU Kiel

A number of techniques have been reported on fabrication of tunnel junction nano structures through anodization in the last decade , . The dimension of such structures can be miniaturized and controlled through the anodic voltage while anodizing. A TiO2 tunnel junction of controlled thickness is similarly produced through anodic oxidation of Ti nanowires produced in a fracture approach . By using an electrochemically grown TiO2 as a gate oxide, we demonstrate nanowire field effect transistors (NWFET) which can be further used as oxygen sensor. Although FET based sensors are undoubtedly of great importance for microelectronics smart sensors, there are limited sensor reports on FET sensor. Gas detection based on this technique relies largely on change of the metal work function in the Schottky diode or MOSFETs induced by catalytic reaction on the solid surface . Here, the oxygen sensing properties are also demonstrated.

MM 28.3 Wed 10:45 IFW D

Phonon absorption at low temperature - determination of the indirect band gap in FeSi using Fourier-spectroscopic infrared ellipsometry — •Dirk Menzel[1], Paul Popovich[2], Alexander V. Boris[2], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The determination of the band gap is an important parameter for the characteristics of a semiconductor. However, for FeSi the size of the gap is not reported consistently so far. Using far-infrared spectroscopic ellipsometry we have reliably determined the dielectric function of FeSi. As predicted by band structure calculations both a direct and an indirect band gap are observed from the absorptive part of the dielectric function which amount to 73 meV and 10 meV, respectively. The absolute value of the indirect gap can only be evaluated when both phonon absorption and emission are observed. At low temperature, however, the former does not occur which generally makes it impossible to obtain the indirect gap energy in the low temperature range. For the ellipsometric measurements we used a Fourier transform spectrometer and, therefore, illuminated the sample with white light. This leads to a continuous generation of optical phonons which may also decay into low-energy acoustic phonons. This method enables one to derive the absolute value of the indirect gap even the low temperature.

MM 28.4 Wed 11:00 IFW D

$Co_xFe_{(x-1)}S_2$: How close to half-metallicity? — •C. Utfeld[1], S. R. Giblin[2], J. W. Taylor[2], J. Laverock[1], S. B. Dugdale[1], C. Shenton-Taylor[3], J. A. Duffy[3], L. Wang[4], C. Leighton[4], M. Itou[5], and Y. Sakurai[5] — [1]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK — [2]ISIS Facility, RAL, Chilton, Oxfordshire OX11 0QX, UK — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, UK — [4]Chem. Eng. & Mat. Sci., University of Minnesota, Minneapolis, MN 55455, USA — [5]SPring-8, 1-1-1 Kouto, Mikazuki, Sayo, Hyogo 679-5198, Japan

CoS_2 is a material thought to be very close to being a half-metal, i.e. to only be conducting in one spin. However, the Fermi level lies low in the conduction bands and doping with the isostructural semiconductor FeS_2 is predicted to gradually unoccupy one spin channel. In this context the evolution of the polarisation across the series $Co_xFe_{(1-x)}S_2$ is of major interest. Experimentally the number of direct measurements accessing the bulk polarisation for different alloy compositions is rather

limited. We present a magnetic Compton scattering study combined with *ab initio* calculations as a method to determine the bulk spin polarisation in CoS_2 and $Co_{0.9}Fe_{0.1}S_2$. Magnetic Compton scattering is a versatile technique for investigations into spin-dependent bulk properties because it probes the unpaired electrons directly. We compare the data with theoretical predictions and optimise the agreement by rigidly shifting the bands in order to extract the *tuned* bulk polarisations of P≈-75% and P≈18% for the pure and the x=0.1 system, respectively.

MM 28.5 Wed 11:15 IFW D

Photoemission insight into heavy-fermion behavior at the nanoscale — •Denis Vyalikh[1], Steffen Danzenbächer[1], Yuri Kucherenko[2], Cornelius Krellner[3], Christoph Geibel[3], Serguei Molodtsov[1], and Clemens Laubschat[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institute of Metal Physics, National Academy of Sciences of Ukraine, UA-03142 Kiev, Ukraine — [3]Max-Planck-Institut für Chemische Physik Fester Stoffe, Nothnitzer Strasse 40, D-01187 Dresden, Germany

We unraveled the hybridization phenomenon between f- and d- states at the Fermi level in the $YbRh_2Si_2$ (YRS) heavy-fermion material. The intriguing point is that upon electron doping the hybridization strength can be systematically tuned. It is demonstrated that gradual deposition of silver atoms onto atomically clean YRS-surface leads to charge transfer from the Ag 5s into the Rh 4d bands substantially changing the energetical overlap of these states and, consequently, the hybridization strength. Another fascinating point is that silver atoms do not penetrate deep inside the crystal, consecutive forming well ordered monolayer's structure. It is an evidence that observed tunable hybridization appears only in the surface region. Then it should reveal its own properties, like heavy-fermion behavior, which can be rather different from the bulk.

MM 28.6 Wed 11:30 IFW D

Relative Sub-shell Photoionization Cross-sections of Selected Metals Determined by Hard X-ray High Kinetic Energy Photoemission — •Mihaela Gorgoi, Franz Schäfers, Walter Braun, and Wolfgang Eberhardt — BESSY II Elektronenspeicherring, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Deutschland

Recently, hard x-ray high kinetic energy photoelectron spectroscopy has lead to a break-through due to its non destructive way of investigating the bulk electronic properties of materials. However, due to the relatively new development of this technique there is a lack of information concerning the photoionization cross section at high energies. Whenever compound materials are investigated or when estimating signal levels and the feasibility of an electron spectroscopy experiment the knowledge of cross sections is essential. Thus in the present work we will show the experimentally determined relative sub-shell photoionization cross sections of selected metals in the energy range of 2 to 10 keV. Based on previous experimental studies of Kunz et al. [1] Au 4f cross sections were used as reference. The data will be compared with the calculated sub-shell photoionization cross sections and the differences will be discussed. [1] C. Kunz, S. Thiess, B.C.C. Cowie, T.-L. Lee, J. Zegenhagen, Nuclear lnstruments and Methods in Physics Research A 547, 73-86 (2005).

MM 29: Diffusion and Point Defects II

Time: Wednesday 12:00–13:00 Location: IFW D

MM 29.1 Wed 12:00 IFW D

Einzelfehlstellennachweis mit dem Mikrostrahl der Bonner Positronen-Mikrosonde — •Sven-Martin Hühne[1,2], Patrick Eich[2], Matz Haaks[2] und Karl Maier[2] — [1]Institut für Anorganische Chemie, Römerstraße 164, D-53117 Bonn — [2]Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, D-53115 Bonn

Die Positronen-Annihilations-Spektroskopie (PAS) ist eine renommierte Methode zur Untersuchung von Kristalldefekten. Für PAS-Messungen ist die Bonner Positronen-Mikrosonde (BPM) eine einzigartige Messapparatur zum ortsaufgelösten Nachweis der Fehlstellendichte. Erstmalig ist es gelungen die Ortsauflösung der BPM auf 1 μm zu optimieren.

Durch Anlassen sind in abgeschrecktem Platin kleine Leerstellencluster erzeugt und anschließend mit Positronenstrahldurchmessern von 50 μm und 1 μm untersucht worden.

Mit einem Strahldurchmesser von 50 μm beobachtet man unabhängig von der Position auf der Probe einen konstanten Linienformparameter, d.h. eine räumlich konstante Fehlstellendichte im Messvolumen. Wird der Strahl hingegen auf 1 μm fokussiert, beobachtet man die statistische Verteilung der wenigen von den Positronen erreichbaren Fehler im Messvolumen. Damit lässt sich zeigen, dass mit Positronen als Sondenteilchen eine einzelne Fehlstelle beobachtbar ist.

MM 29.2 Wed 12:15 IFW D

Calculations of positron annihilation properties for sub-nano precipitates in Al-Mg-Cu alloys — •Björn Korff[1], Iris Kohlbach[1], Benedikt Klobes[1], Torsten Staab[2], Matz Haaks[1], and Karl Maier[1] — [1]Helmholtz-Institut für Strahlen- und Kernphysik Universität Bonn — [2]Fraunhofer Institut für Silicatforschung Würzburg

Early stages of precipitation in age-hardenable aluminum alloys affect the final strength of the alloys by the formation of certain kinds of nuclei. Even though consisting of just a few atoms, these nuclei determine the further growth of precipitates responsible for hardening the alloy.

For their structural analysis we use positron annihilation spectroscopy. In this way we obtain information about the local atomic structure inside precipitates, but especially around vacancies. The interpretation of measurements is assisted by calculations simulating measurable positron annihilation parameters for different possible atomic configurations.

Positron measurements of alloys with aging times from a few minutes to eight hours are compared with calculations for several structures representing candidates for first nuclei of precipitation. This way we learn about the agglomeration of Mg and Cu mediated by the diffusion of quenched-in vacancies and about their arrangement prior to the formation of larger stable structures.

MM 29.3 Wed 12:30 IFW D

Untersuchung von Plastizität und Ermüdung technischer Aluminiumlegierungen mit Positronen — •Marius Wirtz, Patrick Eich, Matz Haaks und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Mittels der Positronen-Annihilations-Spektroskopie (PAS) ist es möglich, die Fehlstellenkonzentration in einem plastisch verformten Material zu bestimmen, was mit der Bonner-Positronen-Mikrosonde (BPM) sogar mit einer Ortsauflösung im Mikrometerbereich möglich ist. Die Positronen dienen hierbei als Sondenteilchen, die sehr empfindlich auf Fehlstellen im sie umgebenden Kristallgitter reagieren. Diese Tatsachen wurden genutzt um die Entwicklungen der Fehlstellendichte in den technischen Aluminiumlegierungen AA2024, AA6013 und AA6082 im Verlauf eines Zugversuchs zu untersuchen. Es konnte gezeigt werden, dass je nach Zusammensetzung und Temperaturbehandlung der Legierungen, der Anstieg der Fehlstellendichte entweder kontinuierlich war oder ab einem bestimmten Punkt von dynamischen Erholungsprozessen im Material überlagert wurde. Darüber hinaus wurde die Fehlstellendichte der Legierung AA6082 unter Wechselbelastung ebenfalls mit Hilfe der ortaufgelösten PAS gemessen und die Ergebnisse zum Abschätzen der Bruchzyklenzahl genutzt.

MM 29.4 Wed 12:45 IFW D

Decomposition phenomena in Al alloys investigated by positron annihilation at low temperatures and XAFS — •Benedikt Klobes[1], Matz Haaks[1], Karl Maier[1], Christiane Rieke[1], and Torsten Staab[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, D-53115 Bonn — [2]Fraunhofer-Institut für Silicatforschung ISC, Neunerplatz 2, D-97082 Würzburg

The decomposition phenomena occurring in AlCu(Mg) and AlMgSi alloys greatly affect their mechanical properties. Usually, these alloys are solution heat treated and quenched. During post-quench ageing

metastable phases are formed which hinder dislocation movement and, thus, constitute the industrial use of these alloys. However, the early stages of decomposition involving agglomerates of few alloying atoms are hard to access experimentally. Therefore, an understanding of the evolution of these stages has not yet been established. Positron annihilation spectroscopy (PAS) has proved its usefulness for the investigation of Al alloys in the last decades and, recently, its sensitivity to the first stages of decomposition. Usually, positrons are attracted by open-volume defects, but utilising the higher positron affinity of nearly all alloying elements in comparison to Al it is possible to probe even defect-free coherent agglomerates by measuring the low temperature dependence of PAS observables. Mainly studying the positron lifetime between 40 and 300 K we attempt to follow the evolution of first agglomerates with and without structural vacancies in AlCu(Mg) and AlMgSi alloys. These results will be correlated with measurements of the x-ray absorption fine structure (XAFS).

MM 30: HV Banhart

Time: Wednesday 14:00–14:30 Location: IFW A

Invited Talk MM 30.1 Wed 14:00 IFW A

Precipitation-hardening of aluminium alloys - challenges and recent developments — •John Banhart — Helmholtz-Zentrum Berlin für Materialien und Energie

Age-hardening of aluminium alloys is an established technology applied on the scale of millions of tonnes annually. Notwithstanding, some fundamental problems associated with the precipitation sequence and kinetics of ageing, even in mass-market alloys, are still awaiting clarification. For example, in many common Al-Mg-Si alloys (6000 series), intermediate storage at or near room temperature after solutionising leads to drastic changes of the precipitation kinetics during the ensuing artificial ageing carried out at much higher temperatures, e.g. 180°C, a result that is not only an annoyance in production, but also counterintuitive and therefore a challenge for researchers. Moreover, the exact precipitation sequence is found to be increasingly more complex than assumed a decade ago. The wealth of structures occurring has only been revealed recently. Recent developments, e.g. in both atom probe microscopy, highest-resolution TEM, small-angle scattering, X-ray absorption spectroscopy etc. have allowed to answer some fundamental questions, but further work is required to provide sufficient understanding that allows for a more target-oriented alloy and process design.

MM 31: Topical Session High Temperature Materials II

Time: Wednesday 14:45–16:30 Location: IFW A

Topical Talk MM 31.1 Wed 14:45 IFW A

Single-crystal nickel-base-superalloys: Correlation between high temperature properties and microstructure — •Thomas Link[1], Alexander Epishin[1], Udo Brückner[2], and Bernard Fedelich[2] — [1]Technical university Berlin, Germany — [2]Federal institute of material reasearch and testing Berlin, Germany

Nickel base-superalloys have a two phase microstructure: a disordered matrix hardened by 70 vol% of ordered precipitates. The strength depends on the properties of both phases but also on their morphology and on the condition of the interface. Dendritic solidification results in dendritic stresses, the different lattice spacings of both phases in coherency stresses. The morphology is described quantitatively and the stresses measured by X-ray diffraction. During high temperature creep deformation the morphology of the ordered phase transforms from cuboids to plates, the coherency stresses relax by interfacial dislocation networks and vacancy generation results in polyedrical pores. These processes are analysed by X-ray-diffraction, SEM, TEM and synchrotron X-ray tomography. Primary, secondary and tertiary creep are analysed by image analysis, TEM and molecular dynamics. Description of the plastic deformation needs microstructurally based models, which consider the evolution of the microstructure during service. A method, to characterise the relevant microstructural parameters is presented. The results of microstructurally based modelling are shown and a brief outlook on material development is given.

Topical Talk MM 31.2 Wed 15:15 IFW A

Atomic site location by channelling enhanced microanalysis (ALCHEMI) in gamma-prime strengthened Ni- and Pt-base alloys — Christian Liebscher, Rainer Völkl, and •Uwe Glatzel — Metallische Werkstoffe, Universität Bayreuth, D-95440 Bayreuth

The additions of alloying elements to Ni- and Pt-base alloys influence the micro structure and thereby the creep properties, whereas the mechanism is uncertain. Therefore atomic site location by channeling enhanced microanalysis (ALCHEMI) was used to determine the site partitioning of ternary and quaternary alloying elements in the L12-ordered gamma-prime phase. Two ternary Ni*Al alloys with Cr and Ti additions were investigated. The measured site partitioning showed that Cr and Ti atoms prefer the Al-sub lattice sites. For a ternary Pt*Al*Cr alloy, it was found that Cr atoms occupy Al sites. The influence of Ni as a fourth alloying element in a Pt*Al*Cr*Ni alloy on the site partitioning was also investigated. The detected results give evidence that in the quaternary alloy Cr and Ni atoms prefer the Pt sub lattice. First principles calculations were used to support the experimental data.

MM 31.3 Wed 15:45 IFW A

Temperature dependence of the lattice misfit of rhenium and ruthenium containing nickel-base superalloys — •Steffen Neumeier[1], Sigrid Schwub[1], Florian Pyczak[2], and Mathias Göken[1] — [1]Department of Materials Science & Engineering, Institute I, University Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Institute for Materials Research, GKSS Research Centre Geesthacht, Geesthacht 21502, Germany

To improve the temperature capability of nickel-base superalloys an increasing amount of refractory alloying elements, especially rhenium (Re) and ruthenium (Ru) has been added during the last decades. These 4th generation nickel-base superalloys possess an increased lattice misfit between the γ- and γ'-phase. Since the lattice misfit varies with temperature and its magnitude is decisive for the evolution of the γ/γ'-microstructure during creep deformation the lattice misfit of several experimental alloys with systematically varied contents of Re and Ru was investigated at temperatures up to 1100 °C using high-resolution X-ray diffraction. It was found that the lattice misfit depend strongly on the chemical composition of the alloys and the partitioning behavior of the alloying elements. Measurements of the hardness of both phases by nanoindentation in an atomic force microscope correspond well with the partitioning behavior. Also the temperature dependence of the lattice misfit is modified by Re and Ru. The change of the lattice misfit with temperature is significantly smaller in all Re-containing alloys compared to Re-free alloys and even less pronounced in Ru-containing alloys.

MM 31.4 Wed 16:00 IFW A

Thermodynamic calculations on the Pt-Al-Ni-Cr alloy system — •Johannes Preussner, Rainer Völkl, and Uwe Glatzel — Metallische Werkstoffe, Universität Bayreuth, Germany

Creep, oxidation and corrosion resistant platinum base alloys with room temperature ductility have been developed for high temperature applications. In this talk a thermodynamic modelling of the Pt-Al-Cr-Ni system will be presented with special focus on the Pt-rich side. The Cr-Pt binary system has been reassessed with the CALPHAD method, based on experimental data and first principles calculations. The four ternary alloy systems will be presented and compared with experimental data available. A four sublattice model has been chosen to describe the ordering reactions between the high temperature fcc phase and the low temperature L12 and L10 phases, which are stable at many differ-

ent concentrations throughout a wide range of the Pt-Al-Cr-Ni alloy system.

MM 31.5 Wed 16:15 IFW A

Modelling of topologically close packed phases in Ni-based superalloys based on thermodynamic and kinetic CALPHAD calculations — •Ralf Rettig and Robert F. Singer — Institute of Science and Technology of Metals, Department of Materials Science and Engineering, University of Erlangen, Martensstr. 5, D-91058 Erlangen, Germany

Single crystal Nickel-based superalloys are important high temperature load bearing materials used in particular for turbine blades in industrial gas turbines and aero engines. These materials show unique high-temperature properties up to high homologous temperatures. Nevertheless modern superalloys are often susceptible to brittle topologically close packed (TCP) phase formation. The aim of the current development of gas turbines is to reduce carbon dioxide emission and fuel consumption and therefore to increase efficiency. To achieve that, the firing temperature has to be increased and materials have to be found that are capable of enduring higher temperatures. Prospective candidates are single crystal superalloys with additions of rhenium and ruthenium. In this study computer modelling based on thermodynamic and kinetic CALPHAD calculations is used to systematically explore the mechanisms of phase stability regarding TCP phase formation in complex single crystal superalloys containing rhenium and ruthenium. Methods are developed for quantitative prediction of TCP phase fractions in dependence of time, temperature and alloy composition and an evaluation with experimental results is presented.

MM 32: Topical Session High Temperature Materials III

Time: Wednesday 16:45–18:00 Location: IFW A

Topical Talk MM 32.1 Wed 16:45 IFW A

The formation and growth of Secondary Reaction Zones in coated 4th generation Ni-base Blade Alloys — •Catherine Rae and Aya Suzuki — Department of Materials Science and Metallurgy, Cambridge, CB2 3QZ, UK

Secondary Reaction Zone (SRZ) formed under aluminized and Pt-aluminised coating have become an increasing problem in advanced single crystal superalloys. The distinctive morphology grows by a discontinuous precipitation reaction similar in many ways to recrystallisation, and destroys the distinctive fine $\gamma\gamma$' microstructure. In thin sections of HP turbine blades this can reduce the load-bearing cross section of a blade by as much as 10%. The morphologies and growth kinetics of the Secondary reaction zones formed between the Plat-Aluminised coating and 4th generation Ni-base superalloy substrates have been investigated. Three alloys were studied with systematically varying Ru content in the range of 2-5 wt%. At the lowest Ru content sporadic formation of SRZ was observed, whilst the higher Ru-containing alloys formed a continuous SRZ within the first hour of exposure at 1100°C. These alloys also showed more rapid SRZ growth, regardless of the original surface finish. EBSD analysis revealed that the higher Ru-containing alloys nucleate many more grains of the SRZ and this leads to a deeper penetration depth into the substrate. Orientation relationships between the coating and the SRZ reveal possible nucleation routes for the SRZ grains. These have been investigated using Focussed Ion Beam sectioning and the extraction of sections for TEM analysis.

MM 32.2 Wed 17:15 IFW A

Load rate dependence of the mechanical properties of thermal barrier coating systems — •Nikolay Zotov[1], Marion Bartsch[2], and Gunther Eggeler[1] — [1]Institut für Werkstoffe, Ruhr Universität Bochum, 44780 Bochum — [2]Institut für Werkstoff-Forschung, DLR Köln, 51147 Köln

Thermal barrier coatings (TBC), composed of yttrium-stabilized zirconia (YSZ) ceramic top coat (TC) and intermetallic NiCoCrAlY bond coat (BC) are commonly used as protective coatings of Ni-based high temperature gas engine components. Nanoindentation techniques are increasingly applied for determining the TBC mechanical properties on a nanometre scale. However, little is known about the load-rate dependence of the mechanical properties, which is important for better understanding of cyclic thermal fatigue experiments. Nanoindentations with different load rates omega were performed on polished cross-sections of TBC, deposited by EB-PVD on IN625 substrates (S), using a XP Nanoindenter (MTS) equipped with Berkovich diamond tip. The Young's modulus (E) of the TC is independent of omega, while E for the BC and the S decreases with omega. The hardness (H) of the TC and the BC increases, while H for the S decreases with omega. From the dependence of H on omega, creep power-law exponents c = 0.24(11) and c = 0.023(6) for the TC and the BC were determined. For all TBC components, a decrease with omega of the power-law exponents n and m, describing the loading and unloading nanoindentation curves, is observed.

MM 32.3 Wed 17:30 IFW A

Micro bending tests on EB-PVD YSZ thermal barrier coatings — •Carolin Pfeiffer[1], Mathias Göken[1], and Ernst Affeldt[2] — [1]Lehrstuhl Allgemeine Werkstoffeigenschaften WW I, Institut für Werkstoffwissenschaften, Universität Erlangen-Nürnberg, Martensstrasse 5, 91058 Erlangen — [2]MTU Aero Engines GmbH, Dachauer Str. 665, 80995 München

Thermal barrier coatings (TBCs) are widely used for protection of turbine components from high temperatures. Since the application of thermal barrier coatings can reduce the substrate temperature by up to 200°C, the gas inlet temperature has risen accordingly and the TBCs have become critical for engine operation. The mechanical properties and the microstructural evolution during operation are essential for the estimation of remaining lifetime of the coating. However, the understanding of this subject is still not sufficient.

In order to investigate the mechanical properties of the ceramic thermal barrier, a bending test rig has been developed which is capable of testing small specimens in a four-point bending mode. The tests are monitored with a high resolution camera, which allows a non-contact determination of the sample deflection by digital image correlation.

The sample material has been heat treated at various temperatures for a range of times, in order to determine the sintering effect on the materials properties. In addition, the material is examined by compression and nanoindentation, in order to study the influence of the size of the tested volume on the values obtained.

MM 32.4 Wed 17:45 IFW A

Oxygen vacancies in yttria-stabilized zirconia: defect configurations and charge states — •Volker Haigis, Felix Hanke, and Matthias Scheffler — Fritz-Haber-Institut, Berlin

Yttria-stabilized zirconia (YSZ) is a standard material for thermal barrier systems, where it is used to shield critical parts of combustion engines from high temperature environments. This application of YSZ is due to its low thermal conductivity and its phase stability over a wide temperature range [1]. Doping of zirconia (ZrO_2) with yttria (Y_2O_3) introduces oxygen vacancies which play a crucial role in stabilizing the technologically relevant tetragonal structure. In spite of some work on structural properties [2], the current understanding of the material at the atomic scale is sparse. Here, we characterize the oxygen vacancies, including their charge states, defect configurations, and concentration in YSZ in an oxygen atmosphere. Relevant defect arrangements are identified, and the respective Gibbs free energies are calculated using *ab initio* atomistic thermodynamics. In addition to standard density functional theory, the GGA+U method is used to analyse the stability of vacancy charge states. We construct a phase diagram giving the thermodynamically stable configurations as a function of the Fermi level, temperature, and oxygen pressure. It is discussed whether non-stoichiometric compositions (more or less than one vacancy per two yttrium atoms) are to be expected at finite temperatures and pressures, and hence under technologically relevant conditions.

[1] A.G. Evans *et al.*, J. Eur. Ceram. Soc. **28**, 1405 (2008)
[2] A. Eichler, Phys. Rev. B **64**, 174103 (2001)

MM 33: Phase Transitions I

Time: Wednesday 14:45–16:30 Location: IFW B

MM 33.1 Wed 14:45 IFW B

Stoichiometrical trends in differential scanning calorimetry measurements on phase-change materials — •Michael Klein, Malte Linn, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, Aachen, Germany

Phase-change materials are alloys which can be rapidly switched between two metastable states, the amorphous and the crystalline phase. At the same time they show pronounced contrast in their electrical and optical properties. They are widely used as the functional layer in rewritable optical discs. Prototypes of electrical devices employing phase change materials as non-volatile memory are already entering the market.

Here we present calorimetric measurements, mainly on ternary Ge-Sb-Te alloys. Scratched-off thin film samples were heated in a differential scanning calorimeter to measure the transition from as-deposited amorphous to metastable crystalline phase and finally to the stable crystalline phase. The different transition temperatures will be analysed as a function of stoichiometry in order to improve the understanding of their interconnection.

MM 33.2 Wed 15:00 IFW B

Crystallization kinetics in materials for PCRAM — •Andreas Kaldenbach, Martin Salinga, Carl Schlockermann, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase-Change RAM is one of the most promising candidates for next generation electrical memory devices. One of its key features is the non-volatility of the stored data, which is due to a permanent structural rearrangement in the used phase change materials: the switching between a highly resistive amorphous state and a low resistance crystalline one. Although already utilized in memory applications, the fundamental mechanism of crystallization kinetics in these materials is still not fully understood. A continuous investigation of the temperature dependence of crystal nucleation and growth is very challenging, since crystallization speed of phase change materials is extremely fast at temperatures between glass transition temperature and the melting point. Until now, this difficulty has been bypassed by extrapolating data taken near the glass transition temperature or close to the melting point, where crystallization is rather slow.

The described experimental gap will be closed by a currently developed setup combining optical and electrical measurements to investigate the crystallization kinetics on a nanosecond timescale. It uses a pulsed laser to thermally induce the switching and a probe laser to measure the changing reflectivity during the switching process. Experimental results from the new setup will be compared with existing theories.

MM 33.3 Wed 15:15 IFW B

High energy photoemission of Heusler shape memory compounds Ni2MnGa and Mn2NiGa — •Catherine A. Jenkins[1,2], Andrei Gloskovskii[2], Jürgen Winterlik[2], Hidefumi Maeda[3], Claudia Felser[2], and Gerhard H. Fecher[2] — [1]UC Berkeley, USA — [2]University Mainz, Germany — [3]Ryukoku University, Japan

High energy photoemission [1] is demonstrated as a tool for observing the structural and magnetic phase transition in magnetic shape memory compounds based on the Heusler structure. Ni2MnGa has been known for more than a decade as a ferromagnetic shape memory compound able to undergo transitions of up to 10% strain in properly oriented crystals. Ferrimagnetic Mn2NiGa [2] has recently been found to undergo up to 20% magnetic field assisted strain in the bulk. Recent work at SPring8 in Japan in bulk single and polycrystals of Ni2MnGa and Mn2NiGa show clear transformations in the valence band. Comparison of the measured spectra to Wien2k calculations are discussed.

[1] G.H. Fecher et al, J. Electron. Spectrosc. Relat. Phenom. 156-8 (2007) 97-101. [2] Barman and Chakrabarti, PRB April 2008.

MM 33.4 Wed 15:30 IFW B

Near-surface microstructure of Ni-rich Ni-Pt — •Markus Engelke[1], Bernd Schönfeld[1], and Philip Willmott[2] — [1]LMPT, Department of Materials, ETH Zurich — [2]SLS, Paul Scherrer Institut, Villigen

While the surface structure and the local atomic arrangement in the bulk of Ni-Pt alloys have been repeatedly studied, not much is known about the intermediate regime accessible by grazing incidence diffraction. Here, Ni-23.2 at.% Pt (110) was investigated at 923 K under UHV using synchrotron radiation at an angle of incidence of 0.75 times the critical angle of total reflection. Diffuse scattering shows maxima of about 5 Laue units at 100 positions. From the diffuse scattering registered at positions in-plane and out-of-plane, Warren-Cowley short-range order parameters were recovered. The assumption of a cubic as well as a tetragonal structure for data evaluation results in similar features; dominant values for nearest and next-nearest neighbors and signs of the parameters as expected for $L1_2$ type of local order.

MM 33.5 Wed 15:45 IFW B

Keine Hinweise auf die adaptive Überstruktur $NiPt_7$ — •Bernd Schönfeld[1], Markus Engelke[1] und Andrei Ruban[2] — [1]LMPT, Departement Materialwissenschaften, ETH Zürich — [2]KTH Stockholm, Schweden

Die diffuse Streuung einer einkristallinen Ni-87,8 at.% Pt Probe wurde mit Röntgenstrahlung ausgemessen. Die Probe wurde bei 603 K ausgelagert, um einen thermischen Gleichgewichtszustand einzustellen. Aus der diffusen Streuung wurde der Beitrag der Nahordnung separiert, der schwache Maxima von etwa 2 Laue-Einheiten an 100-Positionen zeigt. Effektive Paarwechselwirkungen wurden mit der inversen Monte-Carlo-Methode bestimmt. In Monte-Carlo-Simulationen kann damit bei tiefen Temperaturen die vorgeschlagene adaptive Überstruktur $NiPt_7$ nicht eingestellt werden. Vielmehr zeigen die Simulationen eine Phasenseparation in $NiPt_3$ und eine Pt-reiche Matrix. Das Auftreten von $NiPt_3$ mit $L1_2$ Struktur konnte zudem anhand von Überstrukturreflexen einer Probe mit niedrigerer Pt-Konzentration experimentell bestätigt werden. Weiterhin ergeben Elektronenstrukturberechnungen keine Hinweise auf $NiPt_7$.

MM 33.6 Wed 16:00 IFW B

An atomistic study of low-C tetragonal Fe-C states — •Alexander Udyansky, Johann von Pezold, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The tetragonal states of interstitial Fe-C solid solutions are known as martensite, a metastable product obtained by quenching high-temperature austenitic *fcc* solutions with high C content. Along such a processing route, the tetragonality is proposed to be due to Bain's *fcc–bcc* diffusionless transformation. It has been long speculated that the tendency towards tetragonal distortions is an inherent property of the Fe matrix, i.e., it should manifest itself also at low C concentrations, independently on the processing route. To address this issue we calculated the chemical contributions of the interatomic interactions using EAM-potentials [1] and the strain-induced long-range interactions within the microscopic elasticity theory. Our study predicts tetragonal states to be preferred also at low C concentrations due to thermodynamically driven [2] orientational ordering of carbon interstitials. These states are found stable only below their order-disorder transition temperature. Above this temperature the loss of the orientational ordering results in the experimentally observed cubic ferritic phase.

1. T.T. Lau, C.J. Först, et al., PRL 98, 215501 (2007).
2. M.S. Blanter, A.G. Khachaturyan, Phys. Stat. Sol. A 51 291 (1979).

MM 33.7 Wed 16:15 IFW B

Fluence dependence of ultrafast transitions in Arsenic and Antimony — •Nils Huntemann, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

We extend a previous theoretical study [E. Zijlstra et al., New J. Phys. **10**, 033010 (2008)], in which we have predicted that a solid-solid phase transition from the A7 to the simple cubic phase can be induced by a laser in arsenic under pressure, to higher fluences up to 23 mJ/cm^2. This leads to a considerably decrease in the pressure that needs to be applied, namely from 23.8 GPa to 4.0 GPa, and for this reason reduces the experimental effort required for a confirmation.

We further investigate the structural changes of antimony under pressure, which has the same ground-state structure as arsenic, but

undergoes transitions to different phases in interaction with femtosecond laser pulses.

The possibility of ultrafast, laser-induced melting for both materials after excitation is also discussed.

MM 34: Liquid and Amorphous Metals I

Time: Wednesday 14:45–16:30 Location: IFW D

MM 34.1 Wed 14:45 IFW D

On systematics of the atomic structure of liquid and amorphous elements along the periodic table — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

Over many years we systematically studied structure formation at very early stages, within the amorphous state. This state, as well as the liquid one are the precursors of any crystalline state. But, both are not really disordered, instead show a well defined spherically-periodic order (SPO), in the mean around any atom. This order can be seen as a precursor of planar order which is expressed by Bloch's theorem. The SPO is an effect of a self-organizing resonance between global subsystems as there are all the valence electrons on one side, and the forming static structure on the other. We learned that both subsystems may adjust to eachother for an optimal phase stability.

Here we report, starting with hydrogen (Z=1), on systematics in the static atomic structure of liquid and amorphous elements all along the Periodic Table of the Elements, up to bismuth (Z=83), highers are mostly unknown. With the *Resonance Model* we are able to explain major structural features of all the elements, independent whether they are metallically, covalently or van-der-Waals-like bonded, of atomical or molecular type. Main features of unknown structures as for e.g. liquid W, Ta, Mo can be predicted.

MM 34.2 Wed 15:00 IFW D

Supercooled and glass-forming liquids as Skyrmionic textures — •Andrei A. Leonov[1,2], U.K. Rössler[1], and A.N. Bogdanov[1] — [1]IFW Dresden — [2]Donetsk Institute for Physics and Technology

The concept of Skyrmionic textures in chiral magnetic systems [1] has been extended to continuum models for glass-forming liquids. These models describe the frustrated tiling of space by incompatible locally preferred clusters within a generalized elastic theory. The field theory for the local order-parameter includes antisymmetric couplings derived from the decurving of ideal template units into flat space[2]. As a qualitative new feature, we propose a softened modulus of the local intensity of the order parameter. The corresponding classical field theory allows for the stabilization of Skyrmionic localized states and extended textures [3]. The notion of a glassy structure as an entangled network of defect lines is replaced by the complex geometry of an elastic and frustrated continuum that can display both "rotation" or twisting and suppression of the ideal local order. The Skyrmions in the simplest version of the frustration models are close, but soft relatives of the hedgehog solutions in Skyrme's original SU(2) symmetric model for nucleons. It is argued that stable Skyrmions are formed at elevated temperatures in molecular liquids and that their condensation into frustrated textures underlies the stability of supercooled and glassy states. — [1] U.K.Rößler, A.N.Bogdanov, C.Pfleiderer, Nature (London) **442**, 797 (2007). [2] S. Sachdev, D.R. Nelson, Phys. Rev. B **32** (1985) 1480. [3] U.K.Rößler, A.N.Bogdanov, J.Non-Cryst.Solids **354**, 4198 (2008).

MM 34.3 Wed 15:15 IFW D

Stokes-Einstein relation in computer simulated bulk glass forming Cu33Zr67 melts — •xiujun han and herbert schober — IFF, Forschungszentrum Juelich, 52425 Juelich, Germany

The validity of Stokes-Einstein (SE) relation in glass forming Cu33Zr67 melts is checked by studying the relationship between viscosity and self-diffusion coefficient with molecular dynamics simulation. The atomic interaction of Cu-Zr is modeled by modified-embedded-atomic method (MEAM). The self-diffusion coefficient is calculated from mean squared displacements (MSD) and the viscosity is evaluated from Green-Kubo equation. It was found that at temperatures higher than 1500K, SE relation is valid. When the temperature is further decreased, SE relation breaks down, which is an indication of dynamical heterogeneity in the melts.

MM 34.4 Wed 15:30 IFW D

Density, surface tension and viscosity of ternary CuCoNi alloys — •Michael Schick, Jürgen Brillo, and Ivan Egry — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany

We selected the ternary system CuCoNi, which is a good candidate for improving the Giant Magneto Resistance (GMR) of conventional CuCo alloys, for investigation of thermophysical properties.

The latter play an important role in the numerical simulation of processing steps, e.g. casting processes. Along two perpendicular cuts through the ternary phase diagram, surface tension, density and viscosity have been determined as functions of temperature.

For surface tension and density measurements the well established electromagnetic levitation technique was used, which allows a containerless processing of the samples and therefore deep undercooling. Viscosities have been measured in our high temperature oscillating cup viscometer.

MM 34.5 Wed 15:45 IFW D

The hydrodynamic limit in liquid titanium: At which length and time scales is it valid? — •Jürgen Horbach and Andreas Meyer — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

A combination of neutron scattering experiments and molecular dynamics (MD) computer simulations is used to analyze the dynamic structure factor of liquid titanium near its melting temperature. First, we show that the simulation is in good agreement with neutron scattering, regarding the self part of the dynamic structure factor, $S_s(q,\omega)$ (with q the wavenumber and ω the frequency). For both methods, we find that the width of the quasielastic line shows a hydrodynamic q^2 dependence for wavenumbers up to about $1.0\,\text{Å}^{-1}$, and thus the self-diffusion constant can be extracted in this q range. Second, MD simulations allow for an accurate calculation of the total dynamic structure factor, $S(q,\omega)$, over the full relevant range of q and ω. The latter function is compared to the analytically known hydrodynamic prediction that requires the shear and bulk viscosities as well as the thermal diffusion coefficient as an input. The latter transport coefficients are directly computed from the MD simulation. The comparison of the hydrodynamic $S(q,\omega)$ with the "exact one" allows for a quantitative determination of the q-ω range where hydrodynamics is valid.

MM 34.6 Wed 16:00 IFW D

Laser induced non-thermal melting of germanium — •Momar S. Diakhate[1], Harald O. Jeschke[2], and Martin E. Garcia[1] — [1]Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany. — [2]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany.

We study the ultrafast non-thermal melting in bulk germanium. By performing molecular dynamics simulations on time-dependent potential energy surfaces and also static frozen phonon calculations, both based on a non orthogonal tight-binding Hamiltonian, we describe the nonequilibrium melting process occurring in bulk germanium under ultrafast laser pulse excitation. The laser parameters are explicitly taken into account. We show that, upon laser heating, all transverse acoustic phonon modes becomes strongly affected and even destabilized, which drives the melting process. We calculate the time-dependence of the structural properties, in particular the structure factor, and predict the time-dependence of different Bragg-peaks. Our simulations yield nonthermal melting of Ge in less than 1ps after laser excitation.

MM 34.7 Wed 16:15 IFW D

Liquid Phase Separation in Gd-Zr and Gd-Ti Melts — •Steffen Schmitz, Hans-Günther Lindenkreuz, Norbert Mattern, Wolfgang Löser, and Bernd Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Phase-separated metallic glasses can be formed in complex alloys involving binary terminal systems with both, negative and positive en-

thalpy of mixing. The miscibility gaps of Gd-Zr and Gd-Ti melts are determined by electromagnetic levitation experiments. If Gd-Ti melts are undercooled below the binodal line samples exhibit the typical coarse phase separated microstructures. On contrary, in Gd-Zr samples quenched on a Cu-substrate both of the two primary phases, i.e. Gd and Zr, occurred in the matrix simultaneously with the eutectic microstructure. Therefore the existence of a metastable miscibility ap is supposed. The findings are compared with CALPHAD calculations of the binary phase diagrams. The consequences for the formation Gd-Zr-Cu and Gd-Ti-Cu metallic glasses by rapid quenching techniques showing phase separation on the nanometre scale are briefly discussed.

MM 35: Poster Session II

Time: Wednesday 16:30–18:30 Location: P4

MM 35.1 Wed 16:30 P4

Theoretical study of geometry dependent I-V characteristics of copper and gold quantum point contacts — •Saeideh Mohammadzadeh[1], Reinhard Streiter[1,2], and Thomas Gessner[1,2] — [1]Center of Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Research Institution for Electronic Nano Systems, ENAS, Chemnitz, Germany

Quantum point contacts have attracted significant attention with continuing miniaturization of nanoscale electronic components for the two past decades. In present work, we study the electronic transport properties of copper and gold quantum point contacts using the non-equilibrium Green's function technique on the density functional tight binding method for modelling the geometry dependent I-V characteristics. The copper and gold quantum point contacts are sandwiched between cognate (001) electrodes and the electronic current is deduced according to the Landauer formulation to study the effect of the quantum point contact length scales and geometry defects on the electronic transport properties. The transmission coefficients, conductance and the voltage drop characteristics are calculated as well.

MM 35.2 Wed 16:30 P4

Conductivity measurements on FeSi and the influence of the stoichiometry on the susceptibility — •Miriam Friedemann, Dirk Menzel, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

Conductivity measurements on FeSi single crystals grown via the Czochralski method were performed and interpreted within a model containing two rectangular bands as well as two parabolic bands. The two gaps which are observed in Raman [1] and Fourier-spectroscopy [2] respectively, have been confirmed. We found evidence for an additional small gap of the size 6 meV which most likely stems from the existence of a small amount of impurity atoms acting as acceptors. The susceptibility of $Fe_{1-x}Si_x$ single crystals with light variance of the ratio Fe/Si = 1 was measured. It shows that the lowest residual susceptibility at low temperatures is achieved with a light Si excess. As evidenced by measurements on samples before and after annealing, the residual susceptibility is also affected by crystal defects.

[1] A.-M. Racu et al., Phys. Rev. B **76**, 115103 (2007).
[2] D. Menzel et al., submitted to Phys. Rev. B.

MM 35.3 Wed 16:30 P4

Raman study of FeSi under high pressures up to 35 GPa — •Ivan Jursic[1], Dirk Menzel[1], Joachim Schoenes[1], and Klaus Doll[2] — [1]Technische Universität Braunschweig, Institut für Physik der Kondensierten Materie, 38106 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Single crystals of FeSi were grown by tri-arc Czochralski technique. These crystals were investigated by Raman spectroscopy in a diamond anvil cell at pressures up to 35 GPa. The experiment was performed at room temperature.

FeSi crystallizes in the B20 structure, i.e. space group $P2_13$. Factor group analysis predicts 9 Raman active phonon modes for this structure. Measurements outside of the DAC allowed the assignment of the vibrations and showed electron-phonon coupling [1]. Only the strong modes could be observed inside the DAC, i.e. two E-mode vibrations at 180 cm^{-1} and 313 cm^{-1} as well as two T-mode vibrations at 195 cm^{-1} and 310 cm^{-1}.

With increasing pressure the frequencies of the vibrations shift to higher values. The observed shift was compared to density functional theory calculations made within a single particle model. The experiment and theory agree reasonable well. There is a small kink observed in the experiment around 15 GPa which can't be attributed to a structural phase transition and is discussed as electron-phonon coupling.

[1] A.-M. Racu et. al. Phys. Rev. B **76**, 115103(2007)

MM 35.4 Wed 16:30 P4

Semiconductor-to-metal transition in FeSi observed using high-resolution photoemission spectroscopy — •Dirk Menzel[1], Markus Klein[2], Klaus Doll[3], Matthias Neef[4], Damian Zur[1], Ivan Jursic[1], Joachim Schoenes[1], and Friedrich Reinert[2,5] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Experimentalphysik II, Universität Würzburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [4]Institut für Mathematische Physik, TU Braunschweig, Germany — [5]FZ Karlsruhe, Gemeinschaftslabor für Nanoanalytik, Germany

High-resolution angle-resolved photoemission spectroscopy was performed on Czochralski-grown FeSi single crystals. Special care was taken during the in-situ preparation of the crystal surface, since the quality and the cleanness of the surface is crucial for the reliability of the obtained photoemission spectra. The experimental data compared to single-particle band structure calculations based on the local density approximation show a strong renormalization of the bands in the vicinity of the Fermi energy due to the self-energy resulting from electronic correlation effects [1]. Temperature dependent photoemission measurements show that the self-energy is strongly $\vec{k}$-dependent at elevated temperatures which is due to scattering of thermally excited charge carriers only at particular crystal momenta. The results obtained by the photoemission investigations evidence that FeSi is not determined by a Kondo scenario but has to be described as a narrow-band semiconductor in which electronic correlations are involved.

[1] M. Klein et al., Phys. Rev. Lett. **101**, 046406 (2008).

MM 35.5 Wed 16:30 P4

Hybridization Phenomena in the Nearly Half-Filled f Shell Electron System $EuNi_2P_2$ — •Steffen Danzenbächer[1], Denis Vyalikh[1], Yuri Kucherenko[2], Cornelius Krellner[3], Christoph Geibel[3], Serguei Molodtsov[1], and Clemens Laubschat[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institute of Metal Physics, National Academy of Sciences of Ukraine, UA-03142 Kiev, Ukraine — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Strasse 40, D-01187 Dresden, Germany

In this contribution we present high resolution angle-resolved photoemission data of the mixed-valent compound $EuNi_2P_2$ that are complimented with band-structure calculations. The study focuses on the behavior of the $4f^6$ final state close to the Fermi energy. Apart from the ^7F_J multiplet splitting as expected for an atomic-like state, this state exhibits additional splittings and dispersions like a valence state. The data are properly reproduced within a calculation that describes the interaction between the $4f$ and valence-band states in the framework of a simplified periodic Anderson model (PAM). The model starts from atomic-like multiplets and considers hopping-interaction to valence-band states. The strength of the interaction of the valence band with $4f$ states depends on band energy, symmetry and partial f character of the valence band states that vary across the Brillouin zone (BZ). Particulary strong interactions between individual terms of the f multiplets and parabolic bands were experimentally found in good agreement with our theory at different points of the surface BZ.

MM 35.6 Wed 16:30 P4

Electron-phonon interaction and spectral weight transfer in $Fe_{1-x}Co_xSi$ — •Paul Popovich[1], Dirk Menzel[2], Natalia Kovaleva[1], Joachim Schoenes[2], Klaus Doll[1], and Alexander Boris[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

The unusual properties of the narrow-gap semiconductor FeSi continue to attract attention of many theoreticians and experimentalists due to its similarities with some rare-earth compounds known as Kondo insulators. We present a comprehensive ellipsometric study on $Fe_{1-x}Co_xSi$ single crystals (x=0-0.2) in the spectral range from 0.01 to 6.2 eV. Direct and indirect band gaps of 73 meV and 10 meV, respectively, are observed in FeSi at 7 K. Four infrared active modes are assigned at 206, 329, 352, and 458 cm^{-1} for FeSi. Two of them are asymmetric at low temperatures, reflecting the phonon-phonon and electron-phonon coupling in the system. As temperature increases, the indirect gap changes sign manifesting semiconductor to semimetal crossover. The corresponding spectral weight gain at low energies is recovered within an energy range of several eV. The present findings imply that the electron-phonon interaction and semimetallic character of FeSi play the dominant role in the broad-band spectral weight transfer and strongly support the model that $Fe_{1-x}Co_xSi$ can be well described in an itinerant picture taking into account self-energy corrections.

MM 35.7 Wed 16:30 P4

A theory for electrical resistivity for amorphous metals — •Golam Mohammed Bhuiyan[1], md. abdur rashid[2], and a. z. ziauddin ahmed[3] — [1]department of theoretical physics, university of dhaka, dhaka-1000, bangladesh — [2]department of physics, university of dhaka, dhaka-1000, bangladesh — [3]department of physics, university of dhaka, dhaka-1000, bangladesh

An attempt has been made to develop a theory for the electrical resistivity for amorphous metals beyond the Ziman's formalism. The starting point of the proposed theory is the Baym's general formula for electrical resistivity. The Baym's theory is then extended within the quasi-crystalline approximation to have two important terms describing the normal and Umklapp scattering. The present theory thus gives a better picture to understand basic scattering processes which are very much involved in the real electronic transport mechanism. The proposed theory will also give better insight to understand resistivity of disordered systems like liquid metals in particular in the supercooled state.

MM 35.8 Wed 16:30 P4

Primary Crystallisation in Al-rich Metallic Glasses at unusually low Temperatures — •Joachim Bokeloh[1], Nancy Boucharat[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe

The initial stage of the primary crystallisation reaction and the glass transition of the marginal metallic glass Al-Y-Fe has been investigated in conventional and modulated DSC, microcalorimetry, XRD and TEM.

A sharp onset of the primary crystallisation was found in microcalorimetry and XRD studies at temperatures 120 K below the primary crystallisation peak observed in conventional DSC.

A systematic MDSC study of annealed samples revealed a wide spectrum of glass transition onsets which show a strong dependence on the annealing temperature and duration. In addition, the glass transition onsets can be linked to the initial stage primary crystallisation.

The observed spectrum of glass transition onsets may be interpreted as experimental evidence for a phase separation that precedes the nucleation and growth of aluminium nanocrystals in the respective al-rich metallic glasses.

MM 35.9 Wed 16:30 P4

New detectors improve the performance of ASAXS beamline B1 at HASYLAB, DESY — •Ulla Vainio, Tom Schubert, Michael Lohmann, Stephan Botta, Thorsten Kracht, and Rainer Gehrke — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

B1 at the DORIS synchrotron at DESY is one of the first anomalous small-angle x-ray scattering (ASAXS) beamlines. Several upgrades will make the beamline again competitive. During 2008 many improvements have been made to the beamline: A new, thicker Si (311) monochromator crystal is now used. A cooling system for the first monochromator crystal was designed and applied. Better alignment of the whole beamline was made, so a smaller beamstop for the primary beam can be used. Automated sample heating programs were implemented to the measurement program, allowing in situ measurements. A PILATUS 100k detector was tested at the beamline. It was shown that PILATUS has at 11 000 eV about ten times better efficiency and much better resolution than the old 2D gas detector. ASAXS measurements showed very good quality. In 2009 the PILATUS detector and a new system allowing for simultaneous SAXS and wide-angle x-ray scattering (WAXS) measurements will be available. A 1D MYTHEN detector can be used as a WAXS detector. All the improvements combined with new Matlab based data processing tools developed 2007 and 2008 allows for speedy and easy SAXS, WAXS and ASAXS measurements that can be analysed on site right after the measurement of the sample.

MM 35.10 Wed 16:30 P4

Preparation and characterisation of graphite particle reinforced $Zr_{48}Cu_{36}Ag_8Al_8$ BMG composites — •Enrico Mund[1], Jayamani Jayaraj[2], Annett Gebert[2], and Ludwig Schultz[1,2] — [1]TU Dresden, Helmholtzstr. 10, 01069 Dresden — [2]IFW , Helmholtzstr. 20, 01069 Dresden

Bulk metallic glasses exhibit good mechanical properties such as high strength and high hardness. The deformation and fracture properties of BMGs are controlled by the initiation and propagation of shear bands. In order to improve further the mechanical properties, manipulation of the shear band propagation is eminent. By creating ex-situ particle reinforced BMG composites the fracture strength and plasticity can be increased. The particles can act as crack-stopper for the shear bands and become barriers for the shear band propagation.
In this work we use graphite particles due to their easy availability and designated properties. A way to fabricate graphite particle reinforced BMG is demonstrated for a selected ZrCuAgAl alloy with a high glass forming ability. Samples are characterised by various analyses methods in comparison to the monolithic BMG. XRD, SEM and DSC examinations show the influence of the graphite particles to the phase evolution upon casting and the thermal alloy behaviour. Compression tests are carried out to clarify the effect of different graphite particle volume fractions on the mechanical properties. Furthermore the influence of different particle size distributions on the mechanical properties is examined. An optimal relation between particle size and volume fraction for a reinforced BMG with increased plasticity will be proposed.

MM 35.11 Wed 16:30 P4

Relaxation behavior and rheologie of amorphous solids in the cooperative shear zone-model — •Moritz Schwabe, Dennis Bedorf, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In the model of the potential energy landscape (PEL) from Stillinger and Weber, it is important to distinguish two different (beta and alpha) relaxations. In the PEL this is described in the change-over to a new local configuration (intrabasin hopping) or to a configuration with a convert potential energy (interbasing hopping). [1] To describe the response of the system in the cooperative shear zone - model to an external stress, a Frenkal-approach is chosen, which shows the decrease of the barrier height in the PEL. [2]

With this background we study the transition from the elastic to the anelastic response of a metallic glass (PdCuSi) via the change of the temperature and the force. To describe this transition from the linear to the nonlinear behavior we will present on the one hand stress-strain curves in the range from ambient temperature to above Tg and on the other hand creep tests with different forces and temperatures. We thank the SFB 602 and the GRK 782 for financial supporting.

[1] John S. Harmon, Marios D. Demetriou, William L. Johnson and Konrad Samwer, Phys. Rev. Lett., 99, p.135502 (2007) [2] William L. Johnson, K. Samwer, Phys. Rev. Lett., 95, p.195501 (2005)

MM 35.12 Wed 16:30 P4

Study of local and global elastic properties by atomic force acoustic microscopy and ultrasonic spectroscopy of a metallic glass — •Hannes Wagner[1], Stefan Küchemann[1], Christian Vree[1], Walter Arnold[2], and Konrad Samwer[1] — [1]I.Physikalisches Institut, Universität Göttingen — [2]Permanent address: Department of Materials and Technology, Saarland University, Saarbrücken

We are looking for local variations of the indentation modulus of a metallic glass. To visualize this effect we use an atomic force acoustic microscope, where the cantilever of an atomic force microscope is excited by a transducer at ultrasonic frequencies while the sensor tip is contacting the sample surface. From various resonance frequencies of this contact we obtain information about the local stiffness. By using the mechanical model of a vibrating cantilever [1] we are able to derive the indentation modulus of the metallic glass.

To investigate the influence of plastic deformation on the potential energy state of bulk metallic glasses, calorimetry and ultrasonic measurements are performed. Wide-band pulses of a bandwidth of 100 MHz are used to excite the 20 MHz transducer in order to get higher time-resolution. They are used to measure sound velocity as a function of plastic deformation. The results provide evidence of activated relaxations modes.

We would like to thank the SFB 602 for financial support.

[1] M. Kopycinska-Müller, A. Caron, S. Hirsekorn, U. Rabe, H. Natter, R. Hempelmann, R. Birringer and W. Arnold, Phys. Chem. 222, 471, (2008)

MM 35.13 Wed 16:30 P4

Quantification of free volume variations of Pd40Ni40P20 bulk metallic glass deformed by room temperature rolling — •Yuanli Xu[1,2], Yue Zhang[1], Jixiang Fang[1], Horst Hahn[1], and Jiangong Li[2] — [1]Forschungszentrum Karlsruhe, Institut for Nanotechnology, Karlsruhe 76021, Germany — [2]Institute of Materials Science and Engineering, Lanzhou University, Lanzhou 730000, China

Mechanical and thermal properties of metallic glasses change significantly with increasing inhomogeneous deformation. This can be attributed to the introduction of localized excess free volume in shear bands. Therefore, the quantification of free volume is of importance for understanding of the structure of the shear bands and the corresponding changes in mechanical and thermal properties of metallic glasses. In the present work, the Pd40Ni40P20 (at.%) bulk metallic glass prepared by suction casting method was deformed to different strains by rolling at room temperature at a constant strain rate. Differential scanning calorimetry was employed to measure the variation of heat capacity with temperature for the undeformed and rolled Pd40Ni40P20 bulk metallic glass. The average value of the reduced free volume was quantitatively calculated from heat capacity for different strains. Compared with the undeformed Pd40Ni40P20 bulk metallic glass, about 23 % excess free volume was introduced into the rolled Pd40Ni40P20 bulk metallic glass at a strain exceeding 90%. These results may be helpful for understanding of the structure of the shear bands in the bulk metallic glasses and the properties of the deformed bulk metallic glasses.

MM 35.14 Wed 16:30 P4

Liquid Cu-Ni-Fe: Molar volume and short range order. — •Jürgen Brillo[1], Ivan Egry[1], Louis Hennet[2], Mirko Kehr[3], and Irina Pozdnyakova[2] — [1]Institut für Materialphysik im Weltraum, Deutsche Zentrum für Luft- und Raumfahrt, Linder Höhe, 51170 Köln — [2]CRMHT, CNRS, 1D, Ave. de la Recherche Scientifique, 45071 Orleans Cedex 2, France — [3]TU Chemnitz, Institut für Physik, Professur Röntgen- und Neutronendiffraktometrie, Reichenhainer Straße 70, 09216 Chemnitz

The molar volume and the atomic short range order were measured for liquid Cu-Ni-Fe binary and ternary alloys.

All experiments were performed containerlessly using the technique of electromagnetic levitation. The molar volume was determined by optical dilatometry and the atomic short range order was obtained from x-ray diffraction experiments carried out at ESRF in Grenoble.

The results are discussed in view of the volumetric mixing behaviour of the system. It was found that the excess molar volumes of the ternary alloys and the binary Cu-Fe alloys are similar and strongly positive while it is negative for Cu-Ni.

This was partly confirmed by the x-ray scattering experiments which exhibit similarities in the short range order of Cu-Fe and Cu-Fe-Ni: In these systems, the nearest neighbour distance, R, is almost identical and does not vary with the composition whereas R is significantly smaller and increases monotonically with the Cu-concentration in Cu-Ni. There are also hints that in Cu-Fe and Cu-Fe-Ni the molar volume is mainly determined by the first shell coordination number.

MM 35.15 Wed 16:30 P4

Investigation of the liquid-liquid miscibility gap in the Cu-Co-Zr-system — •Björn Schwarz, Norbert Mattern, and Jürgen Eckert — Leibniz Institute for Solid State and Materials Research, Dresden, Germany

For a variety of compositions Cu-Co-Zr prealloys were rapidly quenched by splat-quenching and melt-spinning technique. Concerning the chemical homogeneity, phase constitution as well as amorphicity, that are all essentially influenced by a liquid-liquid miscibilty gap found for this system, the samples were investigated by DSC, SEM, HAADF STEM/HRTEM and XRD. Especially those samples partially exhibitng the (Co/Cu)Zr-phase (B2) with martensitic transformation at low temperature show interesting physical properties that were characterized by measurements of the magnetization and electric conductivity.

MM 35.16 Wed 16:30 P4

First-principles study of the structure and composition of Si_3N_4 surfaces and Si_3N_4/TiN interfaces — •Pawel Rodziewicz and Bernd Meyer — Interdisziplinaeres Zentrum fuer Molekulare Materialien (ICMM) und Computer-Chemie-Centrum (CCC), Department Chemie und Pharmazie Friedrich-Alexander-Universitaet Erlangen-Nuernberg

Due to its hardness as well as thermal and chemical stability, silicon nitride is frequently used as substrate and protective coating. Recently, superhard silicon nitride/titanium nitride-based nanocomposite materials have been synthesized which show a hardness similar to that of diamond. In order to obtain a better understanding of the surface and interface properties of these materials, density functional theory calculations have been applied to study the (0001), $(10\bar{1}0)$, $(1\bar{2}10)$, $(10\bar{1}1)$, and $(1\bar{2}11)$ surfaces of β-Si_3N_4. Surface reconstructions and saturation of the broken surface bonds with H, N, NH, and NH_2 have been taken into account. The relative stability of the different surface compositions is analyzed in terms of surface phase diagrams, and Wulff constructions of the equilibrium shape of β-Si_3N_4 crystallites depending on the chemical environment have been obtained. Additionally, first results on the atomic structure and mechanical strength of coherent $Si_3N_4(10\bar{1}0)$/TiN(001) interfaces with different composition will be presented.

MM 35.17 Wed 16:30 P4

Surface topography evolution during ion beam sputtering of Cu — •Maria Lenius[1], Reiner Mönig[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen — [2]Institut für Materialforschung II, Forschungszentrum Karlsruhe

Ion beam sputtered surfaces develop complex patterns that are controlled by the interplay of various mechanisms such as surface diffusion, surface energy minimization, and shadowing effects. The pattern evolution is not fully understood, particularly in crystalline materials where literature investigations on low index Cu surfaces have revealed the importance of crystal orientation in addition to temperature, ion flux and dose.

In this study, the sputter erosion profiles of Cu grains with different crystal orientations have been investigated as a function of 30 keV Ga ion beam incidence and dose in a focused ion beam microscope. The resulting patterns (ripples, 'leaf' structure, or craters with length scales from 10 nm to 1 um) were characterized using SEM, AFM, and EBSD and depend on both crystal orientation and ion beam incidence. A comparison with the faceted structures of thermally annealed Cu surfaces will be performed to understand the role of surface energy on pattern formation. The final goal is to understand which mechanisms control pattern evolution at sputtered crystal surfaces.

MM 35.18 Wed 16:30 P4

Influence of Ga on the melting behaviour of Pb nanoparticles — •Anna Moros, Harald Rösner, and Gerhald Wilde — WWU Münster, Institute of material physics

In recent years there have been many analyses of the melting of Pb nanoparticles embedded in Al, but the corresponding mechanism of melting is still not completely understood. The current research project analyzes Al-1at%Pb samples, which are prepared by melt-spinning. The melting behaviour of Pb nanoparticles was determined by differential scanning calorimetry. In contrast to findings for free particles and in contradiction to many models of size-dependent melting, it was found that the particles melted at 10-30 K above the melting point of the bulk material. Analyses of TEM-images yielded a bimodal size distribution with most of the small particles in the size range between 2-20 nm. The resolved lattice mismatch between the faceted Pb nanoparticles and the matrix is suggested to be the key to understanding the melting behaviour. What happens if the matrix lattice changes due to alloying of other components? For our project we chose Gallium since it is miscible with Al, but immiscible with Pb. First results were obtained on 6at% Ga and 1at%Pb samples. The results by DSC and TEM are discussed with respect to the impact of the lattice mismatch between particles and matrix on the melting point variation.

MM 35.19 Wed 16:30 P4

Electrical characteristics of metal-Nb:STO interfaces —

•Gesine Saucke, Jörg Hoffmann, and Christian Jooss — Georg-August-Universität Göttingen, Göttingen, Germany

Because of the chemical stability and the small lattice mismatch, strontium titanate (STO) is a widely used substrate material for many perovskite oxides. In addition the conductivity can be tuned by doping with Nb from insulting to a low-resistance behaviour. Therefore Nb:STO is not only of particular importance for deposition of perovskites, but also for the fabrication of novel devices like heterostructures, tunnel- or pn-junctions. In order to examine devices like this, it is important to understand the electrical contact to Nb:STO.

In the vicinity of metallic contacts Schottky barriers are formed, which give rise to a highly non-linear current-voltage relation in two-point configuration. However, the interface resistance not only depends on the work function of the involved materials, but also on the detailed defect structure, e.g. related to the deposition method. In this contribution we summarise our results concerning the fabrication of metallic contacts like Ti, Au, Ag on Nb:STO prepared by sputter deposition techniques with respect to pre-treatment of the substrates, choice of electrode materials and additional post annealing steps.

MM 35.20 Wed 16:30 P4

Transmission electron microscopy study of the interface $Pr_{1-x}Ca_xMnO_3$ / $YBa_2Cu_3O_{7-d}$ — •Jonas Norpoth[1], Thilo Kramer[1], Christian Jooss[1], Hiromi Inada[2], and Yimei Zhu[2] — [1]Institut für Materialphysik, Universität Göttingen — [2]Institute for Advanced Electron Microscopy, Brookhaven National Laboratory

Interfaces between highly correlated electron systems may exhibit novel electronic properties that are absent in the isolated materials. Especially, complex oxide interfaces often feature nontrivial electronic behaviour, the understanding of which needs a careful analysis of the relation between interface structure and electronic properties at the atomic scale. In this work we study the interface between the high-T_c superconductor $YBa_2Cu_3O_{7-d}$ and the hole-doped perovskite $Pr_{1-x}Ca_xMnO_3$. Thin film multilayers fabricated with pulsed laser deposition on epitaxial substrates exhibit atomically sharp interfaces as was demonstrated by high-resolution transmission electron microscopy. Electron energy loss spectroscopy indicates electron transfer across the interface from PCMO to YBCO according to a band bending scenario from the difference in the materials‘ workfunctions. Furthermore, short-range interdiffusion of Ca and Y cations is observed. These charge transfer processes establish doping gradients in the interfacial region capable of affecting both the polaronic transport in the manganite and the characteristics of the superconductivity.

MM 35.21 Wed 16:30 P4

Line stress from step edges and its impact on cantilever bending — •Weina Li[1,2], Huiling Duan[2], Maxim Smetanin[1], and Jörg Weissmüller[1,3] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Peking University,Beijing,P.R.China — [3]Universität Des Saarlandes, Saarbrucken

It is well known that the surface of a solid exerts a mechanical force on the underlying volume phase. This force has important ramifications for the behaviour of nanoscale objects. It is quantified by the surface stress, the derivative of a suitably defined surface excess free energy function with respect to the projection of the bulk strain tensor onto the local tangent plane. By analogy, the line elements at solid surfaces, such as triple lines, edges, or steps may also interact mechanically with the bulk. The relevant forces may be derived by taking the derivative of the line tension - an excess in energy per line length - with respect to the strain. Dimensional considerations might suggest that the line stress will emerge as a vector directed along the local line orientation. Yet, it is well known that parallel step edges interact by lateral dipole forces, so that a more general state of stress may be associated with line elements on a surface. Cantilever bending experiments provide sensitive probes for changes in the elastic interaction of the matter at the surface of a solid with the bulk. We discuss how the presence of step edges impacts the bending of cantilevers. Of particular interest are changes in the bending, either due to the creation of steps or due to the change in line stress during electrochemical cycles or reversible adsorption.

MM 35.22 Wed 16:30 P4

In-situ TEM and STM studies of dislocations in nano-scale metal samples — Burkhard Roos[1], •Sönke Schmidt[1], Daniel S. Gianola[2], Gunther Richter[3], Astrid Pundt[1], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Universität Göttingen — [2]Insitut für Materialforschung II, Forschungszentrum Karlsruhe — [3]Max-Planck-Institut für Metallforschung, Stuttgart

Metals at the nano-scale exhibit mechanical properties that are different from those at the macro-scale. The best known effect is the increase in strength with decreasing crystal size. However, present dislocation-based models fail to explain this effect. It is the goal of the studies described here to directly observe dislocations in small volumes in order to understand how they contribute to size dependent mechanical response. Two different experimental approaches are being taken. In the first approach, in-situ TEM is used to observe dislocation nucleation and storage during tensile testing of metal nano-wires. Initial results from ˜100 nm diameter, single crystal Cu whiskers will be presented. In the second approach, in-situ STM will be used to observe the dislocation traces left at the surface of freshly deposited metal films. Results from deformed Cu films will be presented to show the feasibility of this method for providing quantitative information on dislocations during deformation.

MM 35.23 Wed 16:30 P4

Effect of Surface Roughness on the Deformation of Micron-Sized Specimens of Cu — •Matthias Büchsenschütz-Göbeler and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen

A variety of studies on deformed small scale metal specimens (100 nm to 10 μm) have shown that dislocation storage becomes rarer as the crystal size is decreased. This implies that plastic deformation, which is usually controlled by dislocation interactions, changes to a dislocation nucleation limited mechanism in sub-micron samples. In the study presented here, the effect of surface roughness on the mechanical behavior of single crystal Cu pillars is investigated. It is expected that surface roughness at the 10-100 nm length scale will influence the ease of dislocation nucleation and thus the mechanical behavior in sub-micron specimens. One and 4 μm diameter Cu pillars with varying degrees of surface roughness have been fabricated using a focused ion beam and then compressed using a flat punch tip in a nanoindenter. No effect of the ripples on the stress-strain behavior of the columns was observed, suggesting that deformation is not limited by dislocation nucleation at this length scale. Further tests on even smaller pillars are underway.

MM 35.24 Wed 16:30 P4

Zerstörungsfreie Beobachtung der räumlichen Verteilung von elastischen Konstanten in weicher Materie — •Jessica Mende, Marcus Radicke, Ole Oehms und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany

Mit Ultraschall (US), der während einer Spin-Echo-Sequenz in einem medizinischen Tomographen eingestrahlt wird, können verschiedene elastische Konstanten in weicher Materie dreidimensional und zerstörungsfrei dargestellt werden. In Proben mit unterschiedlichen Festigkeiten werden Kugeln aus einer Öl-in-Gelatine-Mischung eingebracht. Die Proben bestehen aus Agar-Agar und Kieselerde. Agar ist ein biologisches Geliermittel. Die Kieselerde dient zur Absorption des US. Die Kugeln besitzen ein höheres Elastizitäts- und Schubmodul als die Umgebung aus Agar-Agar und Kieselerde.

Von den Proben werden Phasenbilder gemacht, die die Phase der Spins in Grauwerten kodiert darstellen. Die Verschiebung innerhalb der Probe durch den Schallstrahlungsdruck ist abhängig von den elastischen Eigenschaften innerhalb der Probe. Die Darstellung der Verschiebung im Bild erfolgt durch ein Paar von magnetischen Feldgradienten. Während einem dieser Gradienten wird der US mit einer Frequenz von ca. 2,5 MHz und einer Länge von 20 ms eingestrahlt. In den Bildern wird eine Phasenverschiebung durch eine Verschiebung auf der Grauskala sichtbar. In Differenzbildern mit und ohne US können Rückschlüsse auf die räumliche Verteilung der elastischen Eigenschaften der Probe und der darin befindlichen Fremdkörper gezogen werden.

MM 35.25 Wed 16:30 P4

Deformations of auxetic periodic strut frameworks — •Holger Mitschke, Klaus Mecke, and Gerd E. Schröder-Turk — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

We study the deformation behaviour, in particular Poisson ratios, of planar periodic strut frameworks with rigid struts connected at flexible joints. We systematically search for yet unknown auxetic frameworks (i.e. with negative Poisson ratio) and to understand the relationship between structure morphology (quantified by integral geometric

Minkowski measures) and deformation behaviour.

These frameworks are defined by their symmetry group with two lattice vectors $\vec{a}$ and $\vec{b}$, the position of joints $\vec{p}_i$ and strut vectors of length l_{ij}. A deformation of an initially rigid network is obtained, if possible, by changing the lattice vector $\vec{a} \to (1+\delta)\vec{a}$ with $\delta \in \mathbb{R}, |\delta| \ll 1$ but maintaining all initial strut lengths l_{ij} and translational periodicity. The Poisson ratio is extracted from the relative change in the resulting new $\vec{b}$. The deformed network is numerically obtained by a multi-dimensional Newton-Raphson method. Here we present an analysis of strut frameworks based on Archimedean tilings and tilings of star polygons [1].

[1] B. Grünbaum and G.C. Shephard, : *Tilings and patterns*, W.H. Freeman, 1987.

MM 35.26 Wed 16:30 P4

High Temperature deformation of Tungsten — •Armin Huber[1], Bernd Eberhard[2], Andreas Spörhase[1], and Ferdinand Haider[1] — [1]Univ. Augsburg — [2]Osram GmbH, Schwabmünchen

To study the high temperature deformation behaviour of tungsten wires at temperatures up to or beyond 2000°C, we constructed a high temperature deformation chamber. The wire is heated by direct current flow, temperature is controlled pyrometrically and the local elongation is measured optically. We present the construction, validation and first results for tensile deformation experiments of tungsten wires as a function of deformation temperature, wire thickness and material composition. These results are compared to results of conventional experiments at lower temperature.

MM 35.27 Wed 16:30 P4

Mechanical properties of LiB_3O_3 at nanoscale — •Irina P. Shakhverdova[1], Peter Paufler[1], Rimma S. Bubnova2[2], Stanislav K. Filatov[3], and Dirk C. Meyer[1] — [1]Institut für Strukturphysik, TU Dresden, 01062 Dresden, Germany — [2]Institute of Silicate Chem., Russian Academy of Sciences, Ul. Odoevvskogo, 24/2, St.Petersburg 199155, Russia — [3]Dept. of Crystallography, St.Petersburg State University, Univ.Emb.7/9, St.Petersburg 199034, Russia

Indentation hardness (H), scratch hardness (H_S) and reduced Young's modulus (E_r) of LiB3O5 single crystal plates with different orientation as well as of glass with the same composition have been investigated using nanoprobes. Microhardness (H_M) tests were done for comparison. Both hardness and Young's modulus of glass appeared smaller compared to corresponding single crystal data ($H \sim$ 7–8 GPa, $H_M \sim 6$ GPa, $E_r \sim$ 70–80 GPa for glass and $H \sim$ 10–15 GPa, $H_M \sim$ 6–11 GPa, $E_r \sim$ 93–155 GPa for single crystal). H, H_S, E_r and the plane of crack propagation proved orientation-dependent. Cracks in the glass sample were not observed up to 0.49 N microindentation load, whereas for the single crystal the cracks appeared already at 0.098 N. In single crystals the observed cleavage planes {211} and/or {412} are oriented nearly parallel to planes of B-O rings. The dependence of scratch morphology on the direction of scratching is demonstrated quantitatively. The coefficient of friction depends on normal load and varies between 0.25 and 0.37. The oscillating friction reflects elementary processes of plastic deformation at nanoscale. Dislocations created during scratching have been detected by etching.

MM 35.28 Wed 16:30 P4

Simulation of phase diagrams of nanoscale particles — •Michael Gährken, Harald Rösner, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149

The phase diagram of nano-sized binary particles changes compared to macroscopic particles. A theoretical model, based solely on the thermodynamic contribution of the inner phase boundery, was already developed for a simple eutectic system and has been modified for systems with limited solid solubility.

The simple eutectic system's thermodynamic properties follow basically an ideal solution behavior in both the liquid and the solid phase, whereas the solid solubility was introduced by a regular solution behavior in the solid phase.

In addition to theoretical analyses, experimental investigations were conducted on binary Sn-Bi nanoparticles that were embedded in an Al matrix. The obtained results from calorimetry measurements are critically discussed in view of the comparison between experiments and idealized model behavior.

MM 35.29 Wed 16:30 P4

Ultra-fast diffusion in severely deformed NiTi and Ti — •Jochen Fiebig[1], Sergiy Divinski[1], Ruslan Valiev[2], Yuri Estrin[3], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische-Wilhelms Universität Wilhelm-Klem Str. 10 48149 Münster, Deutschland — [2]Institue of Physics of Advance Materials, Ufa State Aviation University, 12K. Marx Street 450000 Ufa, Russian Federation — [3]Monash University, Claytoon, Victoria, Australia

Severely deformed materials attain nowadays a growing technological interest due to their advanced properties and property combinations. In the present study, were focus on the diffusion properties of nanocrystaline NiTi produced by high pressure torsion(HPT) and of ultra-fine grained titanium deformed by equal channel angular pressing (ECAP). The radiotracer method was used with the radioactive isotopes ^{44}Ni and ^{44}Ti in combination with the parallel sectioning technique. Our results discover the existence of ultra-fast diffusion pathways in HPT-processed NiTi, especially after certain heat treatments. The diffusion data are analysed in relation to the existence of 'non-equilibrium' grain boundaries in severely deformed materials, but also with respect of the possible presence of a percolating network of nanocracks and nanovoids in severely deformed materials.

MM 35.30 Wed 16:30 P4

Experimental determination of excess energy contributions in nanocrystalline Pd — •Matthias Wegner[1], Markus Ames[2], Jürgen Markmann[2], Jörg Schmauch[2], Gerhard Wilde[1], and Rainer Birringer[2] — [1]Universität Münster, Institut für Materialphysik, 48149 Münster, Germany — [2]Universität des Saarlandes, Technische Physik, 66041 Saarbrücken, Germany

Nanocrystalline materials with grain sizes considerably below 100nm are characterized by significant contributions of grain boundaries and triple lines to the overall energetics. Until today, the magnitude of triple line energies is unknown and even the sign of their excess energy contribution is discussed. In this contribution, a method is indicated that investigates the excess contributions of grain boundaries and triple junctions for inert gas condensed (IGC) Palladium (Pd) with an average grain size of about 10 nm by micro calorimetric and micro structural investigations. Measurements were done simultaneously at room temperature (23 °C) on two identical halves of the same sample in order to correlate both experiments. A reduction of microstrain and grain coarsening accompanied by annihilation of grain interfaces are observed, which lead to a reduction of free energy. The results and the influence of different geometric grain models underlying the analysis are also discussed in the presented work.

MM 35.31 Wed 16:30 P4

Patterning graphene by electron-assisted local oxidation nano-lithography — •Danny Haberer, Thomas Mühl, Mark H. Rümmeli, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research (IFW) Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The research interest in graphene, a single layer of graphite, is mainly driven by its remarkable electronic properties as well as its recent experimental success. Of the various routes for graphene device fabrication, oxygen plasma etching is a successful technique to apply arbitrary designs to this material. We have recently developed a route through which carbon-based materials can be patterned on the nm-scale by electro-oxidation using a scanning electron microscope with the assistance of water vapor (10 to 100 Pa). We show this method can pattern graphene without the need for an additional lithography step as is necessary with plasma etching. Further, we show the patterning of free-standing graphene membranes, which is far more challenging using conventional etching techniques.

MM 35.32 Wed 16:30 P4

Creep measurements on high pressure torsion treated materials — •Jörn Leuthold, Harald Rösner, and Gerhard Wilde — Universität Münster, Institut für Materialphysik, 48149 Münster, Germany

In ultrafine grained and in nanocrystalline materials the small grain size and the presence of defects with high specific excess energy densities lead to modifications of the basic mechanisms that can accommodate externally applied mechanical stresses. Additionally, for plasic deformation, grain boundary controlled mechanisms, such as grain boundary (GB) emitted dislocations and partial dislocations, twinning, GB diffusion and sliding can be more important or even dominant. To study the modified deformation behaviour several copper samples were prepared by high pressure torsion (HPT), a technique to induce high

shear stresses on a specimen to produce fine grained or even nanocrystalline material. A device for creep measurements was built to perform tensile stress-strain-rate tests at room temperature for the measurement of strain-rate sensitivity of the HPT samples. The results are discussed with respect to the modified plasticity mechanisms in ultrafine and in nanocrystalline metals.

MM 35.33 Wed 16:30 P4

Simulating structural and thermodynamical properties of iron nanoclusters — •Denis Comtesse, Alfred Hucht, and Peter Entel — Universität Duisburg-Essen D-47048 Duisburg

Based on molecular dynamics (MD) simulations using EAM potentials we obtain structural and thermodynamical properties of iron nanoclusters and their sintering. The simulations are performed for magic number cluster sizes up to a number of 12431 atoms per cluster. These special sizes are leading to e.g. icosahedral (ICO) clusters with closed atomic shells. In particular we focuss on the shellwise Mackay transformed (SMT) morphology described in Phys. Rev. Lett **99** 083402 (2007). Our EAM potential perfectly reproduces this morphology for clusters with more than 5 closed atomic shells. Because of the MD simulations allowing us to expand the investigation of this morphology to finite temperatures we find a structulral phase transformation from SMT to ICO structure. The transition temperatures are found to grow monotonic with the cluster sizes taken into account. The sintering of SMT and ICO particles is found to induce a transition in the fcc dominated ICO structure to more bcc dominated structure.

MM 35.34 Wed 16:30 P4

On the quality of electrical contacts between carbon nanofibers in composite-materials — •Michael Konter[1], Pablo Carballera[2], Frank Haupert[2], Bernd Wetzel[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2 Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — [2]Institut für Verbundwerkstoffe GmbH, Kaiserslautern, Germany

We have investigated the electric transport properties of composite materials using temperature dependent dielectric spectroscopy (10 Hz - 2 GHz, 40 K - 290 K). The samples consist of epoxy-resin containing up to 2 vol.% carbon nano-fibers. We observe percolation above a threshold of about 0.05vol.%. The dc-conductivity is associated with a polarization process at high frequencies. The latter one stems from an interfacial polarization process at the contacts between the fibers, which act as barriers. The analysis of the data reveals microscopic information on the quality of these contacts. It is poor close to the percolation threshold and improves with increasing concentration of nano-fibres.

MM 35.35 Wed 16:30 P4

Oxygen diffusion in an reaction rate of cobalt nanoparticles stabilized with different ligands — •Britta Vogel, Axel Dreyer, Nadine Mill, Anna Regtmeier, Inga Ennen, Daniel Ebke, Simone Herth, and Andreas Hütten — Department of Physics, University of Bielefeld, D-33615 Bielefeld, Germany

Cobalt nanoparticles with a diameter of 12nm have initially been prepared with TOPO. Subsequently a ligand exchange was carried out to employ different ligands to the nanoparticles while keeping direct comparability. The decrease of the magnetic moment of the nanoparticles corresponds directly to their oxydation. According to a model of Crank for irreversible reaction in a spherical particle the uptake of oxygen in the particles was analyzed. From the fit of the obtained data to the model, information about the diffusion of oxygen in cobalt and cobalt oxide as well as the oxidationrate is deduced. Additionally the temperature dependence is discussed.

MM 35.36 Wed 16:30 P4

Studies on the Phase Diagram of Boron Employing a Neural Network Potential — •Tobias Morawietz[1], Jörg Behler[1], and Michele Parrinello[2] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780-Bochum, Germany — [2]Department of Chemistry and Applied Biosciences, ETH Zürich, USI-Campus, CH-6900 Lugano, Switzerland

The crystalline phases of elemental boron have a structural complexity unique in the periodic table. The complex connection pattern of the icosahedral building blocks forms a formidable challenge for the construction of accurate but efficient potentials.

We present a high-dimensional Neural Network potential for boron, which is based on first-principles calculations and can be systematically improved. The potential is several orders of magnitude faster to evaluate than the underlying density-functional theory calculations and allows to perform long molecular dynamics and metadynamics simulations of large system. By a stepwise refinement of the potential and an application of the potential in metadynamics simulations we show that starting from random atomic positions the structure of α-boron is predicted in agreement with experiment. Further, pressure-induced phase transitions of α-boron are discussed.

MM 35.37 Wed 16:30 P4

Kinetic and thermodynamic aspects of crystallization in the phase-change material $Ge_{15}Sb_{85}$ — •Peter Zalden[1], Vanessa Coulet[2], Christophe Bichara[3], Michael Klein[1], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen — [2]IM2NP - UMR CNRS 6242, Aix-Marseille Université Campus de Saint Jérôme, case 142, 13397 Marseille — [3]CINaM - UPR CNRS 3118, Campus de Luminy - Case 913, 13288 Marseille

Phase-change materials exhibit a very rare combination of properties as they do not only show crystallization on the nanosecond time scale but also show a pronounced change of the optical reflectivity and the electronic resistivity upon crystallization. This property combination is already exploited in rewritable optical data storage and is explored in Phase-Change Memories (PCM), which are considered to be the most promising candidate for future non-volatile electronic data storage.

In this study, structural modifications in sputtered thin films during the transition from the as-deposited amorphous to the crystalline phase are analysed, employing a combination of Differential Scanning Calorimetry and X-Ray Diffraction. This survey includes a systematic study of heat capacities and transition temperatures for different annealing conditions in the amorphous and partially crystallized state. In addition, diffractograms have been recorded ex-situ during different stages of the thermal treatment. These results indicate a segregation of a Ge-rich phase. A comparison to conventional tellurium based phase-change materials is presented.

MM 35.38 Wed 16:30 P4

Simulations of martensitic phase transitions in FeNi- and NiTi-alloys — •Daniel Mutter and Peter Nielaba — Physics Department, University of Konstanz, 78457 Konstanz, Germany

In order to find out possibilities of a realization of shape-memory systems on the nanometer scale, molecular-dynamics simulations were carried out for iron-nickel- and nickel-titanium-alloys with a maximum of about 5000 particles.
The used potentials arise from the embedded-atom method and can be found in the literature (FeNi [1], NiTi [2]).
The origin of shape-memory behavior are the martensitic and austenitic phase transitions between different crystal structures at certain temperatures or external stresses.
In our simulations, we investigated the temperature-driven phase transformations under the following conditions: free or periodic boundary conditions, surfaces of different structures, on which the simulated systems were placed, vacancies in the systems and various alloy compositions.
An evaluation of bond-orientational order-parameters [3] gives detailed information of the local structure during the phase changes.

[1] R. Meyer, P. Entel, *Phys. Rev. B* **57**, 5140 (1998).
[2] W. S. Lai, B. X. Liu, *J. Phys. Cond. Mat.* **12**, L53-L60 (2000).
[3] P. J. Steinhardt et al., *Phys. Rev. B* **28**, 784 (1983).

MM 35.39 Wed 16:30 P4

Crater Formation in Metals Induced by Femtosecond Laser Pulses — •Steffen Sonntag, Johannes Roth, and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

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

Atomic scale images of the ablation process are shown. We discuss the crater formation induced by Gaussian beam profiles, i.e. by TEM00 modes. Ablation and melting thresholds for different metals will be presented.

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

MM 35.40 Wed 16:30 P4

Salt Precipitation in Complexes of Polyethylene Oxide and Alkali Metal Iodides — •Manuel Reschke, Jens Bastek, Nicolaas Stolwijk, and Gerhard Wilde — Universität Münster, Institut für Materialphysik, 48149 Münster

Thermodynamic properties of polymer electrolytes have been the subject of many scientific reports. DSC measurements were performed on $PEO_{20}RbI$ over the temperature range from 0°C to 170°C for different heating rates. The calorimetric curves show an endothermic peak at about 110°C which can be assigned to the precipitation process of the RbI salt out of the polymer matrix. With lower heating rates, the endothermic peak monotonically shifts to a lower temperature. By extrapolation to zero heating rate, the critical precipitation temperature T_C was determined. These T_C values can be compared with earlier data from conductivity measurements and NMR analyses [1]. Salt precipitation in $PEO_{30}CsI$ was observed by X-ray diffraction after quenching of the complex from Temperatures larger than T_C. Current experiments should provide information about the size of the RbI precipitates by detailed analysis of the diffraction peaks.

[1] J. Bastek, Th. Köster, L. van Wüllen, N.A. Stolwijk, Electrochem. Acta. submitted

MM 35.41 Wed 16:30 P4

Aging dynamics at the martensitic phase transition of Au-Cd quantified by XPCS — •L. Müller[1], M. Waldorf[1], C. Gutt[2], A. Madsen[3], G. Grübel[2], T.R. Finlayson[4], and U. Klemradt[1] — [1]II. Physik. Inst., RWTH Aachen Univ. — [2]HASYLAB at DESY, Hamburg — [3]ESRF, Grenoble — [4]School of Physics, Univ. of Melbourne

Aging phenomena of martensites have been discussed controversially for decades. Although they were successfully associated with defect-related diffusion processes in the low temperature phase (Ren and Otsuka, Nature **389**, 579 (1997)), so far no experiments have directly addressed the characteristic time scales associated with nanoscopic structural changes. Using a $Au_{50.5}Cd_{49.5}$ single crystal X-ray photon correlation spectroscopy (XPCS) measurements in diffraction geometry were carried out at ESRF beamline ID10A. High temperature resolution (0.1 K) and stability (±4 mK) were employed to resolve potential slow dynamics in the vicinity of the phase transition, 2D scattering data close to the (001) Bragg reflection were recorded with a sampling time into the detector of 0.2 s at 1.4 s intervals.

For each temperature one-time correlation functions show significant dynamics only near T_c, being fastest at the transition in disagreement with any critical slowing down scenario. Two-time correlation functions reveal a generally non-stationary behavior and also avalanches in the sample. Characteristic timescales were determined as a function of the aging-time by calculating one-time-correlation functions at a specific age. Fits of Kohlrausch-Williams-Watts functions reveal time constants ranging from ≈ 400 s to over 6000 s at largest aging-times.

MM 35.42 Wed 16:30 P4

Physical significance of the flexibility window in zeolites — •Asel Sartbaeva[1] and Stephen Wells[2] — [1]Inorganic Chemistry laboratory, South Parks Road, Oxford OX1 3QR, UK — [2]Department of Physics and Center for Scientific Computing, University of Warwick, Coventry CV4 7AL, UK

We have recently noted that aluminosilicate zeolite frameworks, modelled as a periodic system of corner-linked polyhedra, display a range of densities within which the polyhedra can in principle be made geometrically ideal. Outside this range, distortions are inevitable due to either stretching of bonds or collisions between oxygen atoms on adjacent tetrahedra. The densities of high-silica zeolites at room conditions is found to lie at the low-density edge of the window, indicating that zeolites are maximally expanded structures. We present new evidence, from a theoretical/experimental study of zeolites with ANA topology, that the flexibility window is a valuable guide in explaining the structures and structural phase transitions of zeolites.

MM 36: HV Bennewitz

Time: Thursday 9:30–10:00 Location: IFW A

Invited Talk MM 36.1 Thu 9:30 IFW A

Onset of plasticity as observed by force microscopy — •Roland Bennewitz — INM Leibniz Institute for New Materials, Saarbrücken, Germany

Indentation experiments on many crystalline materials exhibit pop-in events, which have been described as brutal transition from elastic to elasto-plastic response of the surface. The brutality of the event lies in the sudden nucleation and multiplication of a multitude of dislocations. Using very sharp tips of an Atomic Force Microscope to indent atomically flat and clean surfaces of single crystals in ultra-high vacuum, we have been able to detect pop-in events which correspond to a single glide event over one atomic distance. The emerging dislocation lines terminating the glide plane can be observed on the surface around the indentation by high-resolution non-contact force microscopy. We will discuss the observed dislocation structures and the relation between critical load and theoretical shear stress. Some unexpected observations include sudden dislocation motion as late as 50 minutes after indenting the surface.

MM 37: Topical Session High Temperature Materials IV

Time: Thursday 10:15–12:00 Location: IFW A

Topical Talk MM 37.1 Thu 10:15 IFW A

Experimental and computational analysis of the solidification path in TiAl-based alloys — •Ulrike Hecht, Julien Zollinger, Anne Drevermann, and Victor Witusiewicz — Access e.V., Intzestr. 5, 52ß72 Aachen, Deutschland

Research into the solidification behavior of TiAl-based alloys focuses on (i) the sequence of phase formation and the associated microsegregation, (ii) the morphological features of the mushy zone and (iii) the effect of solidification on subsequent phase transformations in the solid state. Here we report on experimental and computational work that addresses the solidification kinetics of niobium containing TiAl-based alloys on the background of thermodynamic data. First, we briefly describe the thermodynamic database developed for the ternary system Ti-Al-Nb. This database was used to calculate the solidification path and the associated microsegregation for lever rule and Scheil-Gulliver conditions. Bridgman experiments and phase field simulations of dendritic growth bring further insight, mainly with regard to back-diffusion. Both methods were used to perform a statistic analysis of microsegregation and its evolution along the mushy zone of Ti-45Al-8Nb and Ti-47Al-7Nb. Experimental and computational results will be compared to one another and discussed with respect to the onset of peritectic *(Ti) formation in Ti-Al-Nb alloys.

MM 37.2 Thu 10:45 IFW A

Microstructure Formation during Solidification in Multicomponent Gamma-Titanium Aluminide Alloys — •Michael Oehring[1], Fritz Appel[1], Jonathan Paul[1], Renat Imayev[2], Valery Imayev[2], Viola Küstner[3], and Uwe Lorenz[1] — [1]GKSS Research Centre, Institute of Materials Research, Max-Planck-Str. 1, D-21502 Geesthacht, Germany — [2]Institute for Metals Superplasticity Problems, Russian Academy of Sciences, Khalturin Str. 39, 450001 Ufa, Russian Federation — [3]Max-Planck-Institut für Metallforschung,

Heisenbergstr. 3, D-70569 Stuttgart, Germany

In order to exploit the potential of gamma titanium aluminide alloys as high-temperature material multicomponent alloys have to be developed that are adapted to industrial processing conditions. TiAl alloys solidifying solely via the beta-phase exhibit characteristic solidification microstructures, which often involve equiaxed instead of columnar structures, weak textures, and modest segregation. These features result from single-phase solidification and the subsequent solid-state transformations. In view of the development of improved cast alloys, the potential of the beta/alpha transformation with respect to microstructural refinement and its dependence on the addition of several alloying elements has been investigated. It was found, that particularly fine and very homogeneous microstructures can be obtained for certain alloy compositions. The microstructural refinement can be attributed to the alloying effect on the kinetics of the beta/alpha transformation and even can be achieved after slow cooling from high-temperature heat treatments.

MM 37.3 Thu 11:00 IFW A

In-situ investigation of crack propagation in γ-TiAl alloys using atomic force, focus ion beam and scanning electron microscopy — •Farasat Iqbal[1], Florian Pyczak[2], and Mathias Göken[1] — [1]Lehrstuhl Allgemeine Werkstoffeigenschaften, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]GKSS Research Centre Geesthacht, Geesthacht

The present study is focused on crack propagation mechanism in Ti-45Al-1Cr & Ti-45Al-5Nb alloys with lamellar microstructure. Atomic force microscopy (AFM) is a versatile technique to study the crack propagation in-situ. AFM was employed to investigate the local deformations near the crack tip. Scanning electron microscopy (SEM) supplements the in-situ observations and was used to get a basic understanding of the crack propagation path over larger distances.A focused ion beam (FIB) was used to investigate the structures and deformation traces underneath the surface.

It is concluded that the $\gamma/\alpha 2$ interfaces act as favorable sites for new interfacial crack nucleation and also for interlamellar crack propagation. Nucleation of new cracks was often preceded by the interaction of deformation twins with interfaces and also by strong shear band activity in the γ-TiAl lamellae visible as significant surface topography in AFM.Mostly the underneath crack path follows the $\gamma/\alpha 2$ interface similar to the situation observed at the surface. The local misorientation measured with Electron Backscattered Diffraction (EBSD) shows γ-lamellae as the region of high deformation as compare to neighboring $\alpha 2$ -lamellae around the crack tip and its surroundings.

MM 37.4 Thu 11:15 IFW A

Estimation of creep rates from short term tensile test relaxations — •Jonathan Paul, Uwe Lorenz, Michael Oehring, Roland Hoppe, and Fritz Appel — GKSS Research Centre, Geesthacht, Germany

In high temperature applications the creep behaviour of TiAl components can be an important issue. In this respect alloy composition and processing are important factors which need to be optimised so that a proper balance of mechanical properties can be obtained. To obtain a large creep property database requires many tests to be performed at different stress levels and temperatures which of course is both time consuming and expensive.

To overcome this requirement during alloy and processing development, a method of estimating the minimum creep rate at a single temperature but at a series of stress levels from a single short term tensile test including repeated stress relaxations has been developed which is presented in this paper. The experimentally measured minimum creep rates are in reasonable agreement with those predicted from stress relaxation.

MM 37.5 Thu 11:30 IFW A

Investigations of γ-TiAl alloys for industrial application — •Gregor Hullin and Mathias Göken — Institute General Materials Properties, University Erlangen-Nürnberg, Erlangen, Germany

The aim of this work is to improve γ -TiAl alloys for application in automotive engines like turbo chargers or valves. Due to the lower density of TiAl alloys of about 4 g/cm3 the acceleration and the responding characteristics of a turbo charger can be improved. Furthermore the amount of harmful substances in the exhaust gases can be reduced by the elevation of the exhaust temperature. These two facts pose a challenge to find a capable TiAl alloy which has the potential to replace already existing Ni-based superalloys as turbine material. The turbine wheels are fabricated by a newly developed precision casting method. Due to this process high cooling rates can be achieved and therefore a very fine fully lamellar microstructure is produced. This structure in comparison to duplex microstructures has best balance of mechanical properties and is therefore appropriate for the use in turbo chargers. The mechanical properties are determined against casting parameters by doing creep experiments, compression and tensile tests. TiAl alloys remain limited in practical use to about 800°C because of the fast growing non-protective intermixed oxide scale. To make these alloys suitable at elevated temperatures a method to improve oxidation resistance is also under study.

MM 37.6 Thu 11:45 IFW A

Hot-Workability of Gamma-Based TiAl Alloys during Severe Deformation — •Ulrich Froebel — GKSS Research Centre, Institute for Materials Research, Max-Planck-Straße 1, D-21502 Geesthacht, Germany

Gamma-based titanium aluminides are intrinsically brittle up to relatively high temperatures. Inhomogeneous microstructures are particularly harmful in this respect, because critical values of constraint stress can develop after very small strains and lead to premature failure of the material. The structural and chemical homogeneity of components is hence extremely important for engineering applications and is most effectively accomplished by thermomechanical processing. The associated degree of microstructural transformation is determined by the imparted energy that triggers dynamic recrystallization. During traditional metal-forming processes such as extrusion and forging, the strain and thus the imparted energy, is inevitably limited due to geometrical constraints. This often leads to insufficient material consolidation, which is manifested by incomplete recrystallization and significant chemical inhomogeneity. Considerably increasing the deformation strain is therefore necessary to improve the homogeneity of components. In this context the feasibility of cyclic axial deformation, where the sample is deformed alternately in tension and compression or cyclic torsional deformation have been investigated. An assessment of the metallurgical potential of these techniques will be the subject of this presentation.

MM 38: Nanostructured Materials II

Time: Thursday 10:15–11:45 Location: IFW B

MM 38.1 Thu 10:15 IFW B

Electrical and mass transport in filled multi-wall carbon nanotubes — •Markus Löffler, Uhland Weissker, Thomas Mühl, Thomas Gemming, Rüdiger Klingeler, and Bernd Büchner — IFW Dresden, (P.O. box 270116, 01171 Dresden,) Germany

Electrical and concomitant mass transport in multi-wall carbon nanotubes (MWCNT) has been studied in a transmission electron microscope using the tip of an in-situ scanning tunnelling microscope. The mass transport has been found to be driven by electromigration and it has been studied in different regimes. Especially, fully reversible mass transport inside a MWCNT as well as current-induced directed MWCNT growth has been observed. The knowledge of the measured electromechanical properties of filled carbon nanotubes presents a starting point for the understanding of growth dynamics as well as for future applications in nanoelectromechanical systems (NEMS).

MM 38.2 Thu 10:30 IFW B

Quantitative composition of a single-walled carbon nanotube sample: Raman scattering vs. Photoluminescence — •Sebastian Heeg, Cinzia Casiraghi, and Stephanie Reich — Freie Universität Berlin, Berlin, Deutschland

The growth processes of Carbon Nanotubes (CNTs) yield samples containing tubes with a large variety of different chiralities. The qualitative composition of the CNTs product has been revealed by Raman

scattering [1] and by Photoluminescence Emission (PLE) measurements [2]. The quantitative composition, however, remains a task in CNT characterization. We adress this problem by comparing the relative PLE intensities of two families of nanotubes with the relative intensities of the according Radial Breathing Modes obtained by Raman scattering. The PLE measurements were performed by dissolving the HiPCO grown nanotubes in aqueous solution using sodium dodecylbenzene sulfonate as surfactant. Raman Spectroscopy was performed by depositing the tubes from the solution on a silicon substrate by spin-coating. The presence of the CNTs was confirmed by atomic force microscopy. We show that the two methods yield significantly different ratios and we compare the results with theoretical predictions.

[1] J. Maultsch *et al.* Radial breathing mode of single-walled carbon nanotubes: Optical transition energies and chiral index assignment. *Phys. Rev B*, 72:205438, 2005.
[2] S.M. Bachilo *et al.* Structure-assigned optical spectra of single-walled carbon nanotubes.*Science*, 298:2361, 2002.

MM 38.3 Thu 10:45 IFW B

Mechanical properties of iron-filled CNTs — •Uhland Weissker, Markus Löffler, Franziska Wolny, Thomas Mühl, Siegfried Menzel, Albrecht Leonhardt, and Bernd Büchner — IFW Dresden, (PF 270116, 01171

Iron-filled carbon nanotubes (CNTs) are promising nanoscale probes for magnetic force microscopy. To achieve high lateral magnetic as well as topographic resolution, a high stiffness of the nanotube is one of the requirements. Iron-filled CNTs combine several advantages. The filling creates a more localized and harder magnetic moment than common coated cantilevers. The CNT shells protect the filling from oxidation and also ensure high mechanical stability. In this work we performed mechanical investigations on iron-filled CNTs by dynamic and static bending. In the dynamic method a high frequency electric field is applied to the CNT in order to excite a resonant oscillation. In the static method a Lorentz force acts on a current-carrying CNT in the presence of a strong magnetic field (2 Tesla), which is provided by the lens system of a transmission electron microscope (TEM). The CNT mounting is carefully considered; it can be modeled as a torsion spring and provides a correction to the calculated Young's modulus. Depending on the CNT diameter, we found a wide variation in the Young's modulus of iron-filled CNTs.

MM 38.4 Thu 11:00 IFW B

Liquid surface model for carbon nanotube energetic — •Ilia Solov'yov, Maneesh Mathew, Andrey Solov'yov, and Walter Greiner — Frankfurt Institute for Advanced Studies, Goethe University, Frankfurt am Main, Germany

We have developed a model [1] for calculating the energy of single wall carbon nanotubes of arbitrary chirality. This model, which we call as the liquid surface model, predicts the energy of a nanotube with relative error less than one percent once its chirality and the total number of atoms are known. The parameters of the liquid surface model and its potential applications are discussed. The model has been suggested for open end and capped nanotubes. The influence of the catalytic nanoparticle, atop which nanotubes grow, on the nanotube stability is also discussed.

The suggested model gives an important insight in the energetics and stability of nanotubes of different chirality and might be important for the understanding of nanotube growth process. For the computations we use empirical Brenner and Tersoff potentials and discuss their applicability to the study of carbon nanotubes. From the calculated energies we determine the elastic properties of the single wall carbon nanotubes (Young modulus, curvature constant) and perform a comparison with available experimental measurements and earlier theoretical predictions.

[1] Ilia A. Solov'yov, Maneesh Mathew, Andrey V. Solov'yov and Walter Greiner, Phys. Rev. E 78, 051601-(1-13) (2008)

MM 38.5 Thu 11:15 IFW B

Clean production of N-doped Singled-walled Carbon Nanotubes by CDV — •Jessica Walkenhorst[1], José M. Romo Herrera[2], Ana Laura Elias[3], Humberto Terrones[3], Mauricio Terrones[3], and Martin E. Garcia[1] — [1]Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Colloid Chemistry Group at Phisico-Chemistry Department & CSIC Associated Unit in Universidad de Vigo, Vigo, Spain — [3]Advanced Materials Department, IPICYT, San Luis Potosí, México

We synthesized pristine and N-doped Single-Wall-Carbon-Nanotubes (SWCNTs) by the CVD technique, involving the spray pyrolysis of a ferrocene solution in ethanol in an Ar atmosphere. When synthesizing N-doped SWCNTs, the solution also contained benzylamine. The aerosol containing the precursors is guided using a quartz tube into a furnace operating at 950 (965) °C; synthesis times of 30-50 min. After the system cooled down the nanotube material was extracted and characterized. We used modified exprimental setups to increase the quality and quantities of the nanotubes produced. In one case, the gas flow upon cooling continues passing through the aerosol generator. In the other case, it passes directly into the quartz tube, thus bypassing the aerosol generator. The different SWCNT materials were mainly characterized using SEM, TGA and Raman spectroscopy. We observed clear differences in the D/G-band ratios, suggesting an increase in the sample's quality where the carrier gas (upon cooling) was directed straight into the tube, bypassing the aerosol generator.

MM 38.6 Thu 11:30 IFW B

Optimization of PECVD growth of individual vertical carbon nanotubes for field emission applications — •Ronny Löffler, Michael Häffner, Helmut Weigand, Monika Fleischer, and Dieter P. Kern — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Carbon nanotubes (CNTs) are interesting for many new applications due to their excellent electrical and mechanical properties, e.g. in the form of vertical CNTs used as field emitters. A promising way to produce uniform vertically aligned CNTs is the growth by plasma enhanced chemical vapor deposition (PECVD). This process is mainly affected by catalyst material and size, gas mixture and flow, deposition temperature, applied power and growth time. The effect of these parameters on the growth of CNT forests has already been reported by others. We present a variation of parameters focused on the growth of individual CNTs, which react much more sensitively to changes in the deposition process. By systematic variation, optimal growth parameters have been identified for the PECVD growth of individual vertical CNTs to be used as field emitters. The growth process has been integrated into the lithographical fabrication of an electrically controlled test structure for I-V-measurements in a UHV chamber.

MM 39: Phase Transitions II

Time: Thursday 12:00–13:00 Location: IFW B

MM 39.1 Thu 12:00 IFW B

Calculation of Phase Diagrams by Monte Carlo Simulation with Lattice Relaxation — •Rolf Anders and Ferdinand Haider — Universität Augsburg, Institut für Physik

A method for the calculation of phase diagrams for alloys given by EAM potentials is presented. It is based on a Monte Carlo (MC) simulation in which the type of a single atom is changed in each step. After an accepted MC step the atomic coordinates in the vicinity of the modification are relaxed in order to account for elastic effects.

The phase diagram is determined by running simulations at different temperatures and chemical potentials. The resulting equilibrium concentrations reveal the stable phases, whose structure is then analysed by calculating the radial distribution functions for each kind of pair of atoms.

Results are shown for Fe-Ni and Fe-Cu.

MM 39.2 Thu 12:15 IFW B

Atomistic simulations on polymeric nitrogen — •Jani Kotakoski and Karsten Albe — Institut für Materialwissenschaft, TU Darmstadt, Germany

Existence of polymeric nitrogen was proposed in 1992 by Mailhiot and co-workers [Phys. Rev. B 46, 14419]. Despite significant effort, the

structure was synthesized first time a decade later in 2004 by Eremets et al. [Nature Mater. 3, 558]. Interest in this material is due to its enormous energy capacity (more than 140 kJ/mol or 2.0 MJ/g) - 500 times higher than for TNT, for example. This gives promise for applications such as environmentally safe rocket fuel. The material is obtained by applying high pressure and temperature on the conventional molecular nitrogen.

Even though the cubic gauche structure is considered as a school book example of the predictive power of ab initio calculations, it's far from the complete answer for high pressure phases for nitrogen. In fact, within the last few years, more than twenty different new structures have been proposed. We present density functional theory calculations for the free energy of different phases at large temperature and pressure ranges (energy minimization and phonon density of states calculations). Also presented are the thermodynamically most stable (and dynamically stable) phases at intermediate (188-320 GPa) and high pressures (>320 GPa) which were found recently. Further, we have developed an analytic bond order potential (and extended it to non-bond interactions) in order to mimic the experimental setup.

MM 39.3 Thu 12:30 IFW B

A Correction to the Interpolation Functions for phase field modeling of three or more phases. — •Abhik Choudhury[1] and Britta Nestler[2] — [1]Institute of Computational Engineering,Karlsruhe,Germany — [2]Institute of Computational Engineering,Karlsruhe,Germany

The use of the phase field method has spread to the solution of a variety of practical problems, where the usage of a number of phase field parameters becomes necessary. One of the requirements in the phase field methodology is the usage of interpolation functions, for interpolating the energy of the system for all values of the phase fields. The usual interpolation functions for phase field simulations involving two phase field parameters cannot be applied as interpolation functions for the case of multiple phases. The reasons for this are elucidated in this investigation. A correction has been proposed to the interpolation functions that are normally used for the binary phase field models. The results of this correction are shown through simulations. In the phase field model for the present investigation, we use the parabolic multi-obstacle potential term for the surface energy. This is popular because of the ease of calibration to the material properties. However, in the model a symmetric linear third order term is incorporated for changing the shape of the bulk free energy density, to limit the stable solutions to strict binary interfaces. The correlation between the corrected interpolation function and the third order symmetric term is investigated.

MM 39.4 Thu 12:45 IFW B

High-Dimensional Neural Network Potential-Energy Surfaces: From Elemental Solids to Multicomponent Systems — •Jörg Behler and Nongnuch Artrith — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Recently, artificial Neural Networks (NN) have been shown to provide accurate high-dimensional potential-energy surfaces for condensed systems. The evaluation of these NN potentials is several orders of magnitude faster than the underlying electronic structure calculations, which enables a routine application in molecular dynamics and metadynamics simulations of large systems. However, so far the applicability of the NN potentials has been limited to elemental systems. By combining the flexibility of the NN methodology with physically motivated terms we are now able to include long-range interactions. This is a necessary prerequisite for studying binary systems like oxides and general multicomponent systems with significant charge transfer. The capabilities of the method are demonstrated for zinc oxide as a benchmark system. We show that structural and energetic properties of various phases are in excellent agreement with reference density-functional theory calculations.

MM 40: Quasicrystals I

Time: Thursday 10:15–11:30 Location: IFW D

MM 40.1 Thu 10:15 IFW D

The hydrodynamic structure factor of quasicrystals — •Andreas Chatzopoulos and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universiät Stuttgart, Germany

A theory of the hydrodynamic structure factor of quasicrystals is developed and exploited. Based on the hydrodynamic equations for icosahedral quasicrystals we introduce the terms of dynamic correlation and response. For a better understanding of phonon and phason dynamics in reciprocal space we determine in a first step the hydrodynamic structure factor in one dimension.
In three dimensions the anisotropic phasonic peak shapes of the static structure factor are reproduced depending only on the ratio of the two phason elastic constants[1].
Then we show the dynamic extension and illustrate the effect of frequency and kinetic coefficient.

[1] M. de Boissieu et al. *Physical Review Letters*, 75(1): 89-92, 1995.

MM 40.2 Thu 10:30 IFW D

Can Kinematic Diffraction Distinguish Order from Disorder? — Michael Baake[1] and •Uwe Grimm[2] — [1]Fakultät für Mathematik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany — [2]Department of Mathematics and Statistics, The Open University, Walton Hall, Milton Keynes MK7 6AA, UK

Diffraction methods are at the heart of structure determination of solids. While Bragg-like scattering (pure point diffraction) is a characteristic feature of crystals and quasicrystals, it is not straightforward to interpret continuous diffraction intensities, which are generally linked to the presence of disorder. However, based on simple model systems, we demonstrate that it may be impossible to draw conclusions on the degree of order in the system from its diffraction image. In particular, we construct a family of one-dimensional binary systems which cover the entire entropy range but still share the same purely diffuse diffraction spectrum.

MM 40.3 Thu 10:45 IFW D

In search of multipolar order on the Penrose tiling — •Elena Y. Vedmedenko[1], Ron Lifshitz[2], and S. Even-Dar Mandel[2] — [1]University of Hamburg, Jungiusstr. 11, 20355 Hamburg — [2]Tel Aviv University, 69978 Tel Aviv, Israel

We use Monte Carlo calculations to analyse multipolar ordering on the Penrose tiling, relevant for two-dimensional molecular adsorbates on quasicrystalline surfaces and for nanomagnetic arrays. Our initial investigations are restricted to multipolar rotors of rank one through four positioned on the vertices of the rhombic Penrose tiling. At first sight, the ground states of odd-parity multipoles seem to exhibit long-range order, in agreement with previous investigations of dipolar systems. Yet, careful analysis performed here establishes that long-range order is absent for all types of rotors, and only short-range order exists. Nevertheless, we show here that short-range order suffices to yield a superstructure in the form of the decagonal Hexagon-Boat-Star tiling.
[1] E. Y. Vedmedenko, S. Even-Dar Mandelb and R. Lifshitz, Phil. Mag. 88, 2197 (2008).

MM 40.4 Thu 11:00 IFW D

Scaling Behavior of the Participation Ratio in d-dimensional Quasiperiodic Models based on the Octonacci Sequence — •Stefanie Thiem and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

The characteristics of quasicrystals are determined by the nature of their eigenstates. Studying the scaling behavior of the participation ratio p is a practicable way to obtain the localization properties of these wave functions. We investigate d-dimensional quasiperiodic models based on the octonacci sequence and prove that the scaling exponent is independent of the dimension for these models.

The eigenstates of the octonacci chain are obtained by numerical calculations for a tight-binding model. Higher dimensional eigenstates of the associated labyrinth tiling are constructed then by a product approach from the one-dimensional results, allowing the numerical consideration of large systems up to 10^{11} sites. We give explicit construction rules for the energies E and wave functions $\Phi_{\mathbf{r}}$ in d dimensions.

The participation ratio $p = \frac{1}{V}\left[\sum_{\mathbf{r}} |\Phi_{\mathbf{r}}|^4\right]^{-1}$ is studied in one, two,

and three dimensions. It is a known result that p scales for fractal states with $p \sim V^{-\gamma}$ $(0 < \gamma < 1)$ in the number of sites V. We calculated the scaling exponent γ of the average participation ratio $\langle p \rangle$ over all eigenstates for different dimensions and various strengths of the coupling parameter v $(0 < v < 1)$. These results suggest that $\gamma(v)$ is independent of the dimension d. We also give a mathematical proof for the dimension independence of this scaling exponent using the product structure of the labyrinth tiling.

MM 40.5 Thu 11:15 IFW D

Structures of Colloidal Quasicrystals — •Johannes Roth — ITAP, Universiät Stuttgart, Germany

Quasicrystals and archimedean-like tilings formed by strips of squares and triangles have recently been observed in experiments of colloidal particles on laser-generated quasicrystalline substrate potentials (Nature **454**, 501 (2008)). Restricted square-triangle tilings are also present in a model of binary dipolar colloids. We will present several classes of restricted square-triangle tilings and will study their properties by Monte-Carlo simulations.

In a second part we will discuss the properties of quasicrystalline laser potentials with respect to the number of beams. We find that there are significant differences between the five-fold case generated by linearly polarized light on the one hand and other polarizations or seven-fold symmetry on the other hand. In the first case the trapping sites form a structure close to a quasiperiodic tiling while in the second case there are low lying saddle points and far fewer deep minima.

MM 41: Interfaces II

Time: Thursday 11:45–13:00 Location: IFW D

MM 41.1 Thu 11:45 IFW D

Elastic and plastic properties of special grain boundaries in aluminium — •Rebecca Janisch, Naveed Ahmed, and Alexander Hartmaier — Interdisciplinary Centre of Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, 44780 Bochum, Germany

To investigate the role of grain boundaries during deformation and fracture of polycrystalline materials, we perform an ab-initio density functional study of a series of special grain boundaries in aluminium. The goal is to find relationships between the characteristic mechanical properties of interfaces - such as the work of separation, and the grain boundary sliding resistance - and the grain boundary degrees of freedom. We perform "ab-initio tensile tests"at bulk and bicrystal supercells to determine the effective interface elastic constant, the work of separation, as well as the critical stress and displacement for cleavage. The results will be discussed with respect to the grain boundary character (tilt/twist) and misorientation angle. Information on grain boundary sliding can be gained by studying the γ-surface of the interface, Δ E(τ), with τ being a rigid shift parallel to the grain boundary. The morphology of the γ-surface depends on the periodicity of the interface, and thus again on the grain boundary degrees of freedom, and the nature of the chemical bonds. Several γ-surfaces will be compared and the different influences discussed.

MM 41.2 Thu 12:00 IFW D

Ab-initio calculation of stacking-fault energies in Al-based alloys. — Pim Schravendijk[1], •Thomas Gnielka[2], Christian Elsässer[1], and Peter Gumbsch[1,2] — [1]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg — [2]IZBS, Universität Karlsruhe (TH), Kaiserstr. 12, 76131 Karlsruhe

The energetic stability of planar defects as a function of segregated alloying elements in diluted aluminium alloys is studied via ab initio density functional theory (DFT) calculations with the local density approximation (LDA). Several simple and transition metals are chosen as alloying elements and introduced as a substitutional point defects in low concentration (less than 10 at.-%) in the bulk crystal and at planar defects of face-centered cubic aluminum.

Formation energies of planar defects with point defects are determined as a function of the alloying elements' species and concentration. This requires DFT total-energy calculations, for atomistic supercells of the planar defects and point defects, as well as for single crystals of experimentally known intermetallic phases of the alloying elements with the aluminium host metal.

The procedure is applied to extrinsic and intrinsic stacking faults as well as to twin boundaries, and it provides a practical and straightforward estimation for interface and segregation energies in alloys.

MM 41.3 Thu 12:15 IFW D

Ginzburg-Landau theory of grain boundary premelting — •Robert Spatschek[1,2] and Alain Karma[2] — [1]ICAMS, Ruhr-Universität Bochum — [2]Northeastern University Boston

Grain boundary premelting is a phenomenon that emerges from repulsive forces between two differently oriented grains in a polycrystal. Typically, different types of forces contribute to the interaction, but it turns out that in metallic systems often "structural forces" play the dominant role. They are the consequence of lattice incompatibiliies due to a misorientation or grain shifts, and provoke elastic deformations and the formation of dislocations.

Starting from the classical density functional theory or a phase field crystal model we develop amplitude equations to shed light on the forces between solid-melt interfaces on an analytical and numerical level. We find in particular that these forces are significantly shorter ranged than previously anticipated and predict a grain boundary premelting transition for bcc iron.

MM 41.4 Thu 12:30 IFW D

Surface Tension andWetting in Solder Connections — •André Wedi and Guido Schmitz — Institut für Materialphysik,Westf.Wilhelms-Universität,Wilhelm- Klemm-Str. 10, 48149 Münster, Germany

Wetting is an important pre-requisite of a reliable solder connection. However, it is only an indirect measure for the important specific energy of the reactive interface between solder and base metallization. In order to quantify this energy, we measured wetting angles of solder drops as well as interface tensions between different SnPb solders and organic flux at a reflow temperature of 250°C. For the latter, we used the Lecomte-De-Noüy ring method applying suitable geometric corrections. From the two independent data sets, the important energy of the reactive interface is evaluated based on Young's equation. Remarkably, although both, the tension between solder and flux and the wetting angle, reveal significant dependence on solder composition, the specific energy of the reactive interface remains almost constant in the range of 0 to 40 at% Pb. This indicates that the properties of the reactive interface are essentially controlled by the Cu_6Sn_5 intermetallic reaction product. Since this phase grows during reflow, the wetting angle should develop in time, but in our in-situ measurements of this angle no time dependence is seen. In the talk the consequences of this contradiction to existing models of reactive wetting are discussed.

MM 41.5 Thu 12:45 IFW D

Interface width of immiscible layered elements — •Patrick Stender, Guido Schmitz, Constantin Ene, and Henning Galinski — Institute of Material Physics, WWU Münster

Based on the thermodynamics of inhomogeneous systems, it is expected that the chemical transition at an interface between two immiscible components cannot be atomically sharp. Recently, we could demonstrate by atom probe tomography that interfaces of metallic multilayers are indeed of finite chemical width and that this width depends systematically on temperature in thermal equilibrium. Thus, the observed effect becomes especially important for multilayer periodicities in the nanometer range. In the case of GMR devices, it can be made responsible for thermal degradation.

In our work, the temperature dependence of the chemical width of layer interfaces of the binary systems Ag/Cu and Fe/Cr and the ternary system Cu/Ni81Fe19 is studied by atom probe tomography. Metallic triple and multilayers were deposited using ion beam sputter deposition technique. For all samples, an isochronal annealing was performed. Owing to the outstanding resolution of the atom probe tomography, a significant broadening of the interface is demonstrated on the depth scale between 1 and 2 nm.

Because all three systems are immiscible from a thermodynamic point of view and the derived activation energies are way too small to allow an interpretation by conventional interdiffusion, Cahn-Hilliard

theory is used to explain the observed temperature dependence.

MM 42: Nanostructured Materials III

Time: Thursday 14:00–15:45 Location: IFW A

MM 42.1 Thu 14:00 IFW A

Virtual diffraction of MD-simulated nanocrystalline Pd under compression — •Jürgen Markmann[1,2], Dmitriy Bachurin[3], Peter Gumbsch[3], and Jörg Weissmüller[1,2] — [1]Universität des Saarlandes, FR7.3 Technische Physik, 66123 Saarbrücken, Germany — [2]Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen, Germany — [3]Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen, 76131 Karlsruhe, Germany

Wide angle x-ray scattering (WAXS) is a widely used tool to characterise the microstructure of crystalline materials. During the last few years the means were developed to calculate x-ray spectra out of molecular dynamics simulation data and to use these spectra to analyse the MD structures. This approach has been validated to yield reliable results for well defined structures. Now, more realistic samples were investigated and analysed in-situ during a deformation by uniaxial compression. These samples consist of 100 randomly oriented palladium grains and were analysed for microstructural parameters like lattice constant, grain size, microstrain, and stacking fault density which can be evaluated out of the position and shape of the x-ray reflections. The most interesting finding is the increase of stacking fault density with the onset of plastic deformation. The stacking fault density reduces to zero when the structure is unloaded. This will be discussed togehter with the other microstructural parameters in terms of nucleation, dissolution, and movement of dislocations.

MM 42.2 Thu 14:15 IFW A

Segregation-induced near-surface lattice strain in CuAu nanoparticles — •Darius Pohl[1], Elias Mohn[1], Juri Barthel[2], Karsten Albe[3], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]FZ Jülich, D-52425 Jülich, Germany — [3]TU Darmstadt, D-64287 Darmstadt, Germany

For binary nanoparticles, experimental findings indicate the segregation of one alloy constituent towards the particle surface which leads to a surface-near relaxation of the lattice. Due to a difference in the surface free energies between copper and gold, a gold segregation for nanoparticles is expected. In the case of CuAu nanoparticles, Au segregation towards the surface is suggested to lead to a lattice expansion. Through aberration-corrected HRTEM imaging with minimum delocalisation is achieved, and the position of individual atom columns can be determined with unrivalled precision.

Molecular dynamic (MD) simulations of CuAu nanoparticles are conducted under the constraint that the particle surface is terminated with either Cu or Au. A comparison between HRTEM contrast simulations of the simulated structures and experimental HRTEM images then allows to distinguish between the different possible scenarios. It is hereby proven that single crystal CuAu nanoparticles with a mean diameter of 3 nm exhibit a lattice relaxation due to a segregation of Gold atoms. This finding is in agreement with previous results obtained for multiply twinned FePt nanoparticles and thus corroborates that the surface-near expansion of the lattice is due to a segregation rather than to internal stress within the particle structure itself.

MM 42.3 Thu 14:30 IFW A

Size-dependence melting transformation of nanoparticles confined in an Al-rich glass — •Nancy Boucharat[1], Harald Rösner[2], and Gerhard Wilde[2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Universität Münster, Institut für Materialphysik, Münster

A common way to study the size dependence of the melting transformation is given by incorporating nanoparticles within a matrix. This configuration implies additional contributions related to the nature of the interfaces between the particles and the host matrix which strongly affect the melting process. Thus, the incorporation of nanoparticles within a glassy matrix opens a new angle to revise the size-dependence of melting by limiting the constraints imposed on the particles by the presence of a crystalline matrix with anisotropic lattice mismatch. Here, AlYFe glasses containing immiscible Pb or In additions have been synthesized via rapid solidification. As expected for liquid-liquid phase separation, the Pb-containing samples consist of spherical Pb inclusions homogeneously dispersed within the matrix. In contrast, the In-containing samples show non-crystalline In-enriched regions. Applying a subsequent low-temperature treatment involves the crystallization of spherical particles with sizes smaller than 5 nm, which melt at extremely low temperatures compared to the bulk material. In this context, the melting behavior is discussed with respect to the size dependence and to the energetic contributions from the particle/matrix interfaces.

MM 42.4 Thu 14:45 IFW A

Gold nanoparticles under synchrotron X-rays — •Chang-Hai Wang[1], Chi-Jen Liu[2], Tzu-En Hua[2], Chia-Chi Chien[2], Wei-Hua Leng[2], Shin-Tai Chen[2], Cheng-Liang Wang[2], and Yeu-Kuang Hwu[2] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Institute of Physics, Academia Sinica, Taipei, 11529 Taiwan

Gold particles with length scale less than 100 nm develop unique physical properties and biocompatible features that render extensive applications in nanotechnology. To materialize the functionalities, gold nanoparticles with controlled size, favorable surface properties and size distribution would be a pre-requisite. This work describes a new room-temperature synchrotron X-ray irradiation method to prepare reductant- and stabilizer-free colloidal gold solutions. Typical characterization tools include TEM, UV-VIS, FTIR, XRD and ICP-OES. The influence of processing parameters such as the pH value, exposure time, ionic strength and radical scavenger on the structure of gold nanoparticles was investigated. The mechanisms underlying the X-ray-triggered reduction of gold ions and the formation of gold clusters are discussed in detail. An interesting morphological evolution as a function of exposure time, from cross-linked network-like structure to individual particles, has been discovered. This approach could be easily extended to the preparation of polymer-modified colloidal gold by simply adding the polymer species to the precursor solutions. As an implication for nanotechnology, the interactions between gold nanoparticles and cells are also studied and reported.

MM 42.5 Thu 15:00 IFW A

Temperature dependent vibrational fingerprints of gold nano clusters: a DFT study — •Luca Ghiringhelli and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The study of gold nanoclusters is a flourishing topic, due to its importance for catalysis and the presence of unexpected phenomena (e.g. chirality). Here, we apply the recently developed all-electron ab-initio code "FHI-aims" for the density functional (DFT) study of the relative energies and vibrational properties of known isomers of small Au_n ($n \leq 10$) clusters. In particular, besides the calculations of the traditional harmonic frequencies, we focus on the less common evaluation of the (temperature dependent) vibrational spectrum, via Fourier transform of the velocity autocorrelation function, where the velocities come from DFT based Molecular Dynamics trajectories at given temperatures. We underline differences between harmonic and an-harmonic spectra at different temperatures and compare with available experimental data.

MM 42.6 Thu 15:15 IFW A

Delocalization mechanisms of excess free-volume in nanoglasses — •Daniel Sopu[1], Karsten Albe[1], Yvonne Ritter[1], and Herbert Gleiter[2] — [1]Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, P.O. Box 3640, D-76021 Karlsruhe, Germany

Molecular dynamics simulations are presented which provide a detailed picture of the structure of nanoglasses, a class of material which can be synthesized by consolidating nanometer-sized glassy particles. Our results provide evidence the existence of glass-glass interfaces between

the consolidated particles. These interfaces are characterized by an excess free volume. By comparing simulations for covalently bonded Ge nanoglass and metallic CuZr nanoglass, we find that the delocalization of this free volume is driven by homogeneous plastic flow and by thermally activated diffusion. These results suggest that the overall density, microstructure and atomic structure of nanoglasses can be adjusted by the initial particle size and chemical composition as well as by the annealing conditions.

MM 42.7 Thu 15:30 IFW A

Mechanical alloying of Fe-Cu powders: elaborating the microstructure at various scales — •Catharina Wille[1], Taláat Al-Kassab[1,2], Pyuck-Pa Choi[3], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Universität Göttingen, Germany — [2]Material Science and Engineering, King Abdullah University of Science and Technology (KAUST), effective 15 April 2009 — [3]Korea Institute of Science and Technology, Nano-Materials Research Center

In this contribution, the process of mechanical alloying has been studied for both sides of the binary Fe-Cu system. Ranging from light-optical microscopy on the mm-scale to atom probe tomography (APT) on the Ångstrøm-scale, the morphology could be observed on several orders of magnitude. Since a ductile element (Cu, fcc) and a brittle one (Fe, bcc) were combined, striking differences in morphology were expected and found on all length-scales, depending on the mixing ratio. Results on powders with low concentrations of the respective minority component will be presented and discussed.

Regarding the widespread application and accessibility, Fe-Cu acts as an ideal binary model alloy to elaborate the enforced non-equilibrium enhanced solubility being immiscible and characterised by a large positive heat of mixing. Chemical identification on the Ångstrøm-scale was granted by APT. Thus, not only the atomic mixing of Fe and Cu could be evaluated, but also the distribution of impurities, mostly stemming from the fabrication procedure.

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

MM 43: Liquid and Amorphous Metals II

Time: Thursday 16:00–17:45 Location: IFW A

MM 43.1 Thu 16:00 IFW A

serrated flow behavior in bulk metallic glasses — •gang wang, norbert mattern, and jürgen eckert — Institute of complex materials, IFW-Dresden, 01069 Dresden, Germany

Plastic deformation of bulk metallic glasses (BMGs) is a complex inhomogeneous process characterized by avalanches in the motion of shear bands. In the present study, based on the CuZr-based BMG, we investigate the serrated flow behavior in the plastic deformation stage. We statistically analyze the serrated stress-strain behavior of BMGs with different plastic deformation ability. The cumulative possibility distribution of the elastic energy density follows the Weibull distribution. Accompanying with the compression tests, we measured the atomic-scale strain during the serrated flow stage by x-ray synchrotron radiation at room temperature. High resolution strain scanning reveals the relationship between the macroscopic serrated flow and the atomic-scale elasto-plastic deformation. Based on the potential energy landscape (PEL) theory of ductile glasses, we attempt to construct a clear physic image of the origination of the plastic deformation in glassy phase, i.e. the evolution from the disorder atomic cluster, to shear transforming zone (STZ) formation, to shear bands origination and then to the shear slip occurring.

MM 43.2 Thu 16:15 IFW A

Dynamics of shear localization and stress relaxation in amorphous $Cu_{50}Ti_{50}$ — •Max Neudecker and S. G. Mayr — I. Physikalisches Institut, Georg-August-Universitaet Goettingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Dynamic heterogeneities of atomic mobility in metallic glasses are investigated for the model glass $Cu_{50}Ti_{50}$ with the help of classical molecular dynamics computer simulations. By rapid quenching from melt at various cooling rates (comprising 5 orders of magnitude), differently relaxed amorphous cells are prepared. During subsequent shearing, we observe a series of highly localized shear events, termed shear transformation zones (STZs). Detailed analysis focuses on geometrical shape and size of STZs, mechanical stress dynamics and correlations of mobility with local properties. We identify a local stress bias as physical origin of STZ formation during during low temperature deformation. Further investigations concern the characterization and analysis of heterogeneous mobility and stress dynamics during shearing at higher temperatures.

[1] M. Neudecker and S. G. Mayr, Acta Materialia, in press (2008)

Financially supported by the DFG (PAK 36)

MM 43.3 Thu 16:30 IFW A

Temperature and kinetics of shear band propagation in amorphous metals — •Florian H. Dalla Torre, David Klaumünzer, Alban Dubach, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Wolfgang-Pauli-Str. 10, 8093 Zurich, Switzerland

Deformation in bulk metallic glasses (BMGs) far below their glass transition temperature is known to be spatially inhomogeneous and restricted to narrow nanometer-sized shear bands. In this study the shear band characteristics of Zr-based BMGs has been investigated as function of strain rate and temperature. To capture discrete shear events precisely a dedicated acoustic emission spectrometer has been used in-situ during deformation testing, which allows for extremely high data acquisition rates of the order of MHz. Preliminary results of evaluating the viscosity within shear bands during deformation suggest that the local temperatures are of the same order of magnitude as those measured during homogeneous deformation close to the glass transition temperature. Acoustic emission results indicate that irreversible deformation starts well before reaching the elastic limit and that the Kaiser effect known to crystalline metals is present also in amorphous metals. It is shown that serrated flow and the associated stress drops are a function of temperature and strain rate. The time periods for a shear band to be activated increases with decreasing temperature from milliseconds at ambient temperatures to seconds at temperatures of 200 K.

MM 43.4 Thu 16:45 IFW A

Modelling the mechanical properties of bulk metallic glasses with nanoscale precipitates — •Yvonne Ritter and Karsten Albe — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

Bulk metallic glasses exhibit unique mechanical properties as compared to conventional crystalline metals. Large elastic strains and specific strengths exceeding the strength of crystalline alloys by more than 100% illustrate the high potential for structural applications. On the other hand, metallic glasses have a relatively low tensile ductility and fail catastrophically when reaching the flow stress. Nanoscale precipitates in the glassy matrix were found to improve the plasticity of BMGs. The underlying mechanisms, however, that lead to the improved deformation bahavior have not yet been exposed. In this study, we investigate the role of structural inhomogeneities in CuZr by means of molecular dynamics simulations. Nanoprecipates of crystalline Cu and CuZr as well as amorphous precipitates with varying composition are investigated and their influence on the materials behavior under tensile load and shear is investigated.

MM 43.5 Thu 17:00 IFW A

Deformation-induced martensitic transformation in Cu-Zr-Al(Ti) bulk metallic glass composites — •Ram Bachchan Kumar, Simon Pauly, Jayanta Das, and Jürgen Eckert — Institut für Komplexe Materialien, IFW Dresden

Plastic deformation of Cu-Zr-(Al, Ti) bulk metallic glass (BMG) composites induces a martensitic phase transformation from the B2 to the B19* CuZr phase. Addition of Ti to binary Cu-Zr increases the temperature above which the B2 CuZr phase becomes stable. This affects the phase formation upon quenching in Cu-Zr-Ti BMG composites. The deformation-induced martensitic transformation is believed to cause the strong work hardening and to contribute to the large compressive deformability with plastic strains up to 15%.

MM 43.6 Thu 17:15 IFW A

Elastostatic preloading of bulk metallic glasses — •Denise Beitelschmidt[1], Sergio Scudino[1], Uta Kühn[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institut für Komplexe Materialien, Helmholtzstrasse 20, D-01069 Dresden — [2]TU Dresden, Institut für Werkstoffwissenschaft, D-01062 Dresden

Many bulk metallic glasses (BMG) show excellent elastic properties but their plastic behaviour is poor at room temperature. However recently, it has been reported that elastostatic compression below the yielding point can be used to enhance the plasticity of BMGs. In this work, the effect of preloading in the elastic regime on the structure and mechanical behaviour of different BMGs is investigated. Different alloys are tested with regard to their changing mechanical properties: as-cast and after preloading. Rods have been cast by different mould-casting techniques and were studied concerning their as-cast structural properties. Those as-cast samples have been preloaded for different periods and loads in the elastic regime and the effect on room-temperature plastic deformation has been investigated. Possible structure variation (e.g., SRO, atomic packing etc.) and creation of free volume as a result of preloading have been analyzed by XRD, DSC, density measurements and ultrasonic investigations. The results will be discussed with already published results from other groups to clarify the mechanisms of structural changes by preloading below yield strength.

MM 43.7 Thu 17:30 IFW A

Synthesis and mechanical properties of Al-based alloys prepared by hot extrusion and spark plasma sintering of gas atomized powders — •Kumar Babu Surreddi[1], Hoang Viet Nguyen[2], Miroslava Sakaliyska[1], Fahad Ali[1], Sergio Scudino[1], Vikas C Srivastava[3,4], Volker Uhlenwinkel[3], Ji-Soon Kim[2], Daniel J Sordelet[5], and Jürgen Eckert[1,6] — [1]IFW Dresden, Institut für Komplexe Materialien, Dresden, Germany — [2]Research Center for Machine Parts and Materials Processing, University of Ulsan, Ulsan, Republic of Korea — [3]Institut für Werkstofftechnik, Universität Bremen, Bremen, Germany — [4]Metal Extraction & Forming Division, National Metallurgical Laboratory, Jamshedpur, India — [5]Materials and Engineering Physics Program, Ames Laboratory (USDOE), Iowa State University, Ames, Iowa — [6]TU Dresden, Institut für Werkstoffwissenschaft, Dresden, Germany

Bulk nanocrystalline and ultrafine-grained Al-based specimens were prepared by in-situ devitrification and consolidation of gas atomized glassy powders. Consolidation was carried out at different temperatures by hot extrusion as well as by spark plasma sintering (SPS). Both techniques lead to highly dense bulk specimens with a microstructure consisting of an fcc-Al phase together with several intermetallic compounds. The consolidated materials display high compression strength, which depends on the consolidation technique, together with large plastic deformation. These results indicate that the mechanical properties of the samples can be tuned within a wide range of strength and ductility as a function of the consolidation technique and parameters used.

MM 44: Quasicrystals II

Time: Thursday 14:00–15:00 Location: IFW B

MM 44.1 Thu 14:00 IFW B

In situ observation of the formation of the metastable decagonal quasicrystalline D-phase in Al-Ni melts — •Dirk Holland-Moritz[1], Olga Shuleshova[2], Wolfgang Löser[2], Guillaume Reinhart[3], and Thomas Buslaps[4] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Leibnitz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01171 Dresden, Germany — [3]ESA External Research Fellow, ESRF / ILL, 38042 Grenoble, France — [4]ESRF, 38043 Grenoble, France

The phase selection during solidification of undercooled Al-Ni melts is investigated by time-resolved in situ measurements using a combination of electromagnetic levitation technique and energy dispersive diffraction of synchrotron radiation. For the investigated alloys in the composition range of 18 - 31.5 at.% Ni undercooling below the liquidus temperature does not influence the selection of the primary solid phase even at highest levels of undercooling. If the semi-solid samples are cooled to lower temperatures we were able to undercool the peritectic reaction during which under equilibrium conditions Al_3Ni is formed. If a sufficient undercooling below the peritectic temperature is obtained a metastable phase is formed, that is identified as the decagonal quasicrystalline D-phase. It subsequently transforms and can only be conserved up to room temperatures if sufficiently high cooling rates are applied. Financial support from the European Commission EU within the IMPRESS Integrated Project under contract FP6-500635-2 and the provision of beamtime by ESRF are gratefully acknowledged.

MM 44.2 Thu 14:15 IFW B

Mechanical behavior of Al-based metal matrix composites reinforced with Al-Cu-Fe quasicrystalline particles — •Fahad Ali[1], Sergio Scudino[1], Gang Liu[2], Kumar Babu Surreddi[1], Mira Sakaliyska[1], Vikas C. Srivastava[3,4], Volker Uhlenwinkel[4], and Jürgen Eckert[1,5] — [1]IFW Dresden, Institut für Komplexe Materialien, Dresden, Germany — [2]State Key Laboratory for Mechanical Behavior of Materials and School of Materials Science and Engineering, Xian Jiaotong University, China — [3]Metal extraction & Forming Division, National Metallurgical Laboratory, Jamshedpur, India — [4]Institut für Werkstofftechnik, Universität Bremen, Bremen, Germany — [5]TU Dresden, Institut für Werkstoffwissenschaft, Dresden, Germany

Al-based metal matrix composites reinforced with Al62.5Cu25Fe12.5 quasicrystalline particles have been produced by powder metallurgy. Composites with different volume fractions of reinforcement have been consolidated into highly dense bulk specimens by hot extrusion and the resulting effects on mechanical properties and microstructure have been examined in detail. Considerable increase in compressive strength and Young modulus has been observed in the composites samples as compared to pure Aluminum. Finally, the elastoplastic deformation of the composites containing different volume fractions of quasicrystalline particles have been modeled by using the self-consistent effective medium approach.

MM 44.3 Thu 14:30 IFW B

Charge transfer as well as hybridization effects in amorphous AlCuLi to optimize phase formation — Michael Lang and •Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

We report on structure-forming processes in ternary amorphous AlCuLi which also forms at higher temperatures a quasicrystalline phase, without transition metals involved as in many other quasicrystalline alloys. In those quasicrystals with transition elements we could show earlier that a phase-stabilizing effect based on self-organized resonances between the electronic system and the static atomic structure exists (Peierls-, Hume-Rothery-like), with subsequent pseudogaps at the Fermi edge and hence strong electronic transport anomalies. The resonance was found to be enhanced by hybridization effects of the Al-p-states with the empty e.g. Fe-d states in i-AlCuFe.

Due to the lack of transition elements in the system under consideration, we were looking for other stabilizing effects than a hybridization-enhanced resonance. And indeed, for AlCuLi due to the lithium there exists an enhancement of the resonance stabilization by charge transfer causing ionic bonding features. But, in addition, indications exist that even for the present alloys hybridization effects may exist. We report on the static atomic structure as well as electronic transport over a large range of composition.

MM 44.4 Thu 14:45 IFW B

Mechanical milling of single-phase Al-Cu-Fe quasicrystals — •S. Scudino[1], F. Ali[1], V.C. Srivastava[2,3], N.K. Mukhopadhyay[4], K.B. Surreddi[1], M. Sakaliyska[1], V. Uhlenwinkel[3], and J. Eckert[1,5] — [1]IFW Dresden, Institut für Komplexe Materialien, Dresden, Germany — [2]Metal extraction & Forming Division, National Metallurgical Laboratory, Jamshedpur, India — [3]Institut für Werkstofftechnik, Universität Bremen, Bremen, Germany — [4]Centre of Advanced Study, Department of Metallurgical Engineering, Banaras Hindu University, Varanasi, India — [5]TU Dresden, Institut für Werkstoffwissenschaft, Dresden, Germany

The effect of milling intensity on the microstructure of spray-deposited

Al62.5Cu25Fe12.5 quasicrystals has been investigated. The first stages of milling are characterized by a strong decrease of the grain size and by the introduction of lattice strain. This effect increases with increasing the milling time and in the material milled for longer time the quasicrystals transform into a nanoscale bcc phase. At this stage, the quasicrystals are no longer observable, indicating a complete transformation of the quasicrystals into the bcc phase. The hardness of the milled powders decrease with increasing the milling time, most likely as a consequence of the increased volume fraction of the bcc phase. Finally, the bcc phase formed during milling is metastable and transforms back to the quasicrystalline phase during the heat treatment, which suggests that a composite material with optimized mechanical properties can be produced by an appropriate thermo-mechanical treatment.

MM 45: Phase Transitions III

Time: Thursday 15:15–16:30 Location: IFW B

MM 45.1 Thu 15:15 IFW B

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

The knowledge of short-range order and nucleation behavior in a liquid is of fundamental importance for understanding the crystallization process of metals. To get a valuable insight in this process on the atomic length scale, we chose the way of analyzing a colloidal model system of charged silica spheres in aqueous solution. Its interaction can be controlled in a precise way by varying sodium hydroxide concentration. This colloidal system is characterized by convenient time scales between seconds and minutes and particle distances up to 500nm and is thus accessible by simple, yet powerful optical techniques. In addition to this, USAXS technique was used to determine the short-range order and nucleation behavior far from equilibrium state. These results are compared particularly with regard to those of a metallic system and show similarities which verify the chosen colloidal system as a good model system for metals.

MM 45.2 Thu 15:30 IFW B

Crystal growth in metallic melts: A computer simulation study — •Roberto Rozas Cardenas and Jürgen Horbach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

The crystal growth of Ni is studied using molecular dynamics computer simulation. The interactions between the particles are modeled by a potential of the embedded atom type. To this end, we consider the direct simulation of crystal growth through the movement of a planar solid-liquid interface at different temperatures. The kinetic growth coefficients and the melting temperature are estimated from an analysis of the interface growth velocity. The resulting melting temperature is at 1748 K, close to the experimental one at 1728 K. The crystal growth coefficient is about two orders of magnitude larger than in the intermetallic alloy $Al_{50}Ni_{50}$. We show that in the latter system crystal growth is driven by diffusion in the solid-liquid interface region, whereas for pure Ni phononic degrees of freedom lead to the much faster crystal growth kinetics.

MM 45.3 Thu 15:45 IFW B

Investigation of nucleation in undercooled melts of pure metals — •Stefan Klein[1,2] and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Containerless processing is an effective tool for undercooling metallic melts far below their equilibrium melting temperatures. By using such levitation techniques the dominating heterogeneous nucleation on container walls is completely eliminated. Furthermore, if the experiments are performed under clean environmental conditions, heterogeneous nucleation on free surfaces is also greatly reduced. In this work both electromagnetic and electrostatic levitation techniques are used for a comparative investigation of nucleation in undercooled metallic metals. In case of electromagnetic levitation samples in a diameter of 7mm are processed within high purity inert gas atmosphere while in case of electrostatic levitation samples in a diameter of 2mm are processed in ultra high vacuum. With a modified model by Skripov a statistical analysis of the distribution function of the undercoolings measured in one experiment run consisting of at least 100 undercooling cycles is conducted which provides information about the physical nature of different nucleation mechanism depending on experiment conditions.

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

MM 45.4 Thu 16:00 IFW B

Undercooling and solidification of Ni_2B under different conditions of convection — •Sven Binder[1,2], Jianrong Gao[3], and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Key Laboratory of Electromagnetic Processing of Materials, Northeastern University, Shenyang 110004, China

We investigate the kinetics of crystal growth by measurements of the dendrite growth velocity as a function of undercooling during non-equilibrium solidification. Measurements are conducted under different conditions of convection. The liquid samples are levitated and undercooled in strong alternating electromagnetic fields leading to forced convection. Inductive stirring is avoided by processing the samples in a liquid or glassy slag where only natural convection is present. Forced convection and natural convection can be reduced by performing undercooling experiments in reduced gravity. The experimental results obtained under different conditions are compared to each other in order to investigate the influence of convection on the growth dynamics of dendrites in undercooled melts. The congruently melting compound Ni_2B is chosen as sample system. It forms an intermetallic phase with growth velocities that are comparable to the fluid flow velocities in electromagnetically levitated melts. The results are analyzed within dendrite growth models and reveal that the growth velocity is essentially influenced by forced convection in strong electromagnetic fields. The present work is supported by DFG under contract HE1601/22.

MM 45.5 Thu 16:15 IFW B

Crystal growth in undercooled NiZr melt: Linking phase-field modeling to molecular dynamics simulations — •Mohammed Guerdane[1], Denis Danilov[1], Frank Wendler[1], Helmar Teichler[2], and Britta Nestler[1] — [1]Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Germany — [2]Institute of Materials Physics, University of Göttingen, Germany

Propagation of a planar solidification and dissolution front in a two-phase crystal-melt structure under non-equilibrium conditions (supersaturated solution) is considered by molecular dynamics (MD) simulations and phase-field modeling (PFM). The MD simulations are carried out with interatomic potentials for the NiZr alloy and provide the thermophysical data required for setting up the PFM simulations. Results are presented showing a comparison of concentration profiles across the crystal-melt interface and of the growth velocity obtained from MD and PFM methods. By considering different approximations of the free energy density in the PFM, we analyze the contribution of the activity coefficient in the chemical potential and of the solute-solvent interdiffusion in the growth dynamics.

MM 46: Electronic Properties II

Time: Thursday 16:45–18:00 Location: IFW B

MM 46.1 Thu 16:45 IFW B

The Korringa-Kohn-Rostoker method: its mathematical foundations — •Robert Hammerling — Center for Computational Materials Science, TU Wien, 1060 Wien — Wolfgang Pauli Institute, Uni Wien, 1090 Wien

The Korringa-Kohn-Rostoker(KKR) method is a well-established method in condensed matter physics to calculate the static Green function of a one-body Schrödinger operator. The multi-site problem is split in a single site problem and the evaluation of the free Green function under appropriate boundary conditions. While both ingredients individually are well understood the resulting expression for the multi-site Green function is still questioned in the mathematical physics community. In this work the mathematical foundations of the KKR method are critically examined.

MM 46.2 Thu 17:00 IFW B

Structural and magnetic properties of Fe under pressure — •Sergey Mankovsky, Jan Minar, Svitlana Polesya, and Hubert Ebert — Dept. Chemie und Biochemie/Phys. Chemie, Universität München, München, Deutschland

The structural bcc→hcp phase transition in Fe under pressure has been investigated on the basis of ab-initio electronic structure calculations using the KKR Green's function method. The role of the magnetic order on the stability of the bcc structure was studied. For this purpose an analysis of the total energy and magnetic structure was performed at different pressure values along a transformation path connecting the bcc and hcp structures. This allows an explanation of the small differences in pressure dependent structural and magnetic XAS signals observed experimentally. In addition, calculations of phonon spectra at different pressure values have been performed. They are based on the formalism of the calculation of the real-space force-constant tensor within the KKR Green's function method. An analysis of different contributions to the dynamical matrix shows the responsibility of the exchange splitting of spin-up and spin-down energy bands for the stabilisation of bcc structure at low pressure.

MM 46.3 Thu 17:15 IFW B

A theoretical description of spin resolved transport — •Stephan Lowitzer[1], Diemo Ködderitzsch[1], Hubert Ebert[1], and Julie B. Staunton[2] — [1]Department Chemie und Biochemie, LMU München, Butenandtstraße 11, 81377 München — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Spin resolved transport became during the last years a fast growing field of interest for many theoretical working groups. We present an approximative scheme to calculate the spin decomposed conductivity within the Kubo-Greenwood formalism. The electronic structure calculations are based on the fully relativistic Korringa-Kohn-Rostoker (KKR) band structure method in connection with the coherent potential approximation (CPA) alloy theory. To demonstrate the reliability of our approach we apply this formalism to $Fe_{1-x}Cr_x$ and the diluted magnetic semiconductor system (DMS) $Ga_{1-x}Mn_xAs$.

MM 46.4 Thu 17:30 IFW B

First-principle study of the connection between structure and electronic properties of gallium — •Elena Voloshina[1], Krzysztof Rosciszewski[2], and Beate Paulus[1] — [1]Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany — [2]Institute of Physics, Jagiellonian university, Reymonta 4, 30059 Krakow, Poland

Different structures of gallium have been studied by means of density functional theory (DFT). The density of states of orthorhombic α-Ga, the only elemental solid exhibiting both metallic and molecular character at zero pressure, shows a pseudogap at the Fermi energy. Complex analysis of the relation between lattice structure and the corresponding electronic properties allows us to throw a light upon an origin of the pseudogap. We have found that the free-electron-like behavior which is a property of the high-pressure *bct* and *fcc* phases of gallium depends strongly on the arrangement of atoms in the buckled planes, one of the building blocks of the orthorhombic gallium.

MM 46.5 Thu 17:45 IFW B

Quantum effects on the Elasticity of Graphene: An ab-initio and tight binding study — •Soumya Bera[1], Andreas Arnold[1], and Ferdinand Evers[1,2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

One of the most interesting aspect of single layer graphene is its surface corrugation (ripples), which can either be intrinsic or induced by surface roughness of the substrate. The long wavelength elastic properties of this novel material are also of great interest and we investigate them here. Our focus is on elasticity in the presence of ripples. We are going to employ two distinct methods namely ab-initio and tight binding calculations, in order to study the effect of ripples together with there associated zero modes on elasticity.

Our ab-initio study supports the exceptional quadratic dispersion relation of flexural(out-of-plane) phonons which is imposed by the spatial symmetries in the long wavelength limit of elastic theory. While short wavelength optical phonons have been studied in the past, to the best of our knowledge our work is the first ab-initio study on the long wave-length context. This DFT analysis also suggests a considerable amount($\sim 4\%$) of change in elastic constants due to zero point motion of phonons originated from the in-plane strain in the system. Using a tight binding model with nearest neighbor hopping we are now exploring the impact of zero energy states on elasticity. Here the source of these zero energy states is strain, induced by ripples.

MM 47: Liquid and Amorphous Metals III

Time: Friday 10:15–12:00 Location: IFW A

MM 47.1 Fri 10:15 IFW A

On physical properties and the atomic structure of Al-Pd alloys — •Nan Jiang, Jan Rauchhaupt, and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

In recent years we reported on an electronic influence on phase stability of Al-3d-TM alloys (TM: Sc, ..., Cu). The electronic influence is based on an internal exchange of momentum between global subsystems, namely the electronic system and the forming static structure. Both systems come into resonance to each other. The resonance is enhanced by a hybridization effect between the Al-p- and the empty TM-d-states causing a reduced effective electron density of the total system. Structure formation, phase stability and the evolution of electronic transport properties were found to be strongly related. In the present contribution we start to replace systematically the 3d-TM elements by the 4d-TM.

For thin films of amorphous Al-Pd alloys, deposited in situ at about 4 K, the resistivity and the thermopower are measured from 4 K to 350 K, the atomic structure after annealing to 350K. By comparing the strongest diffraction ring at K_{pe} with $2k_{\mathrm{F}}$, the Fermi-sphere diameter, stabilizing resonances are detected, indicating two stable regions, one at around $Al_{66.7}Pd_{33.3}$, where a hybridization effect seems to be most prominent, and another one around $Al_{40}Pd_{60}$ without hybridization.

MM 47.2 Fri 10:30 IFW A

Strukturelle und elektronische Charakterisierung binärer amorpher Al-Sc-Legierungen — •Martin Stiehler[1], Danny Müller[2] und Peter Häussler[1] — [1]TU Chemnitz, 09107 Chemnitz — [2]Roth & Rau AG, 09337 Hohenstein-Ernstthal

Untersuchungen an binären amorphen Übergangsmetall-Aluminiden haben in der Vergangenheit gezeigt, dass Hybridisierungseffekte zwischen Al-p- und ÜM-d-Zuständen einen optimierenden Einfluss auf

die Phasenstabilität besitzen. Dies wurde in einem Hume-Rothery-ähnlichen Bild, dem Resonanzmodell, erklärt, bei dem der Durchmesser der Fermi-Kugel mit dem Durchmesser der Pseudo-Brillouin-Zone übereinstimmt und so zu einem stabilisierenden Pseudogap führt. Mit Al-Sc konnten wir die Untersuchung der Legierungsreihe der 3d-ÜM mit Al bezüglich der statischen Struktur und des elektrischen Widerstandes nun abschließen. Durch das daraus folgende Vorliegen von Daten für Systeme sowohl mit *frühen* als auch mit *späten* Übergangsmetallen konnten interessante Ergebnisse bezüglich des Einflusses der Elektronegativitätsdifferenz der Legierungsbestandteile gewonnen werden. Es zeigt sich, dass die Unterscheidung in frühe und späte Übergangsmetalle zumindest für diese Legierungen überdacht und durch eine neue Interpretation ersetzt werden muss. Ob sich die gefundene Systematik auch in anderen Eigenschaften widerspiegelt, müssen ergänzende Untersuchungen zeigen.

MM 47.3 Fri 10:45 IFW A

Thermal stability of Fe-Co-B-Si-Nb glassy alloy — •Trisha Karan[1,2], Shanker Ram[2], Mihai Stoica[1], and Jürgen Eckert[1,3] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]Materials Science Centre, Indian Institute of Technology, Kharagpur 721302, India — [3]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

The thermal stability of Fe-Co-B-Si-Nb glassy alloy is studied by using high temperature differential scanning calorimetery. When the ribbons/rods made from this alloy are heated with a constant heating rate, the glass transition appears as a change in heat capacity and it is followed by one exothermic peak which corresponds to the crystallization process. The glass transition temperature T_g and the crystallization temperature T_x were measured as the onsets of the respective events. Higher the value of T_g and T_x higher is the thermal stability. It was found that in case of continuous heating with a constant rate of 10 K/min the value of T_g and T_x are 808 K and 844 K, respectively. Moreover, a small difference in thermal stability between the rods and the ribbons was observed, which may be due to the different degree of relaxation as a result of different cooling rates reached during solidification. The enthalpy of crystallization, which indicates the stability of super cooled liquid, was found to be -29.72 J/g. Thus, the alloy has good thermal stability and can be used for industrial applications. Additionally, the crystallization behaviour will be discussed.

MM 47.4 Fri 11:00 IFW A

Localization and delocalization of free volume and stress field during structural relaxation of metallic glasses — Jixiang Fang, Horst Hahn, and •Herbert Gleiter — Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe 76021, Germany

Molecualr dynamics (MD) simulation indicated that a delocalization phenomenon can be happened in the nanoglasses. The atomic structures as well as the density (and hence all structure/density-dependent properties) of nanoglasses may be tuned by controlling the degree of delocalization (by modifying the annealing time and/or annealing temperature). Here, we show another system to quantitively characterize the localization and delocalization (i.e, its generation and annihilation) of the additional free volume which may be introduced by a stress field of crystal/glass interface formed via embedding crystals into metallic glasses. In this model, W/CuZrAl and W/PdNiP crystal/glass system were selected to obtain a maximum thermal residual stress for the samples prepared from the melt spinning process. Finite element analysis (FEA) was used to optimize the volume faction of tungsten into glass and to study the stress field distribution. Differential scanning calorimetry (DSC) was adopted to quantitively calculate the average free volume in glass and its variation as annealing under different conditions. The thermal residual stresses for the samples as-quenched and annealed under various conditions were measured by the in situ heating X-rays diffraction (XRD) techniques. Above structural relaxation processes was studied in atomic scale by MD simulation.

MM 47.5 Fri 11:15 IFW A

Structural Change of Zr-Ti-Cu-Ni-Al Metallic Glass with Hydrogen Absorption Treatment — •Jerome Paillier, Annett Gebert, Christine Mickel, Margitta Uhlemann, and Ludwig Schultz — Leibniz-IFW Dresden, Helmholtzstr. 20, Dresden

The use of metallic glasses for mechanical properties-based application is expected because of high yield strength and hardness. Nevertheless, a lack of ability to be strained plastically leading to brittle-fracture behaviour in both tension and compression experiments hinder their development as structural materials. Many routes are contemplated to enhance the toughness of the metallic glasses ; a possibility is to prepare a material with structural/chemical fluctuations on the nanometre scale.

Zr-Ti-Cu-Ni-Al metallic glass alloys have been studied since they exhibit a high-glass forming ability, a wide undercooled liquid region and a high thermal stability. Copper clusters formation within the amorphous matrix is expected to widen the plastic domain of the alloy. For that purpose, hydrogen has been absorbed electrochemically within the alloys. The interaction between hydrogen and the amorphous matrix is complex and dependent on the charging conditions and on the amount hydrogen absorbed. Among others, Cu-rich clusters of 10-15 nm can be formed under certain conditions. The aim is to understand/establish the relationship between the amount of hydrogen absorbed and the evolution of material characteristics. The microstructure changes have been notably characterized by XRD and TEM and also in an indirect way by the change of the thermal properties.

MM 47.6 Fri 11:30 IFW A

Enthalpy relaxation study of Zr45.0Cu39.3Al7Ag8.7 bulk metallic glass and quantification of its free volume by free-volume theory — •Yue Zhang, Horst Hahn, and Herbert Gleiter — Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany

Enthalpy relaxation study of Zr45.0Cu39.3Al7Ag8.7 bulk metallic glass (BMG) is performed at 648, 658, 668, 678 and 684 respectively. It is found that the recovered enthalpy follows the VFT relationship, the fragility parameter D and characteristic temperature T0 are 15.9 and 475K respectively. The activation energy Ea of the glass transition is derived from a modified Kissinger method. Finally, the free volume in the samples is calculated using free-volume theory with D, T0 and Ea as parameters.

MM 47.7 Fri 11:45 IFW A

Corrosion behaviour of the $(Fe_{44.3}Cr_5Co_5Mo_{12.8}Mn_{11.2}C_{15.8}B_{5.9})_{98.5}Y_{1.5}$ bulk metallic glass and its crystalline counterpart — •Petre Gostin, Uwe Siegel, Annett Gebert, Uta Kühn, Jürgen Eckert, and Ludwig Schultz — IFW, Dresden, Germany

The corrosion behaviour of the bulk glassy $(Fe_{44.3}Cr_5Co_5Mo_{12.8}Mn_{11.2}C_{15.8}B_{5.9})_{98.5}Y_{1.5}$ alloy and its crystalline counterpart was assessed by employing anodic polarization tests in combination with microscopy techniques: transmission and scanning electron microscopy and atomic force microscopy. The crystalline counterpart is composed mainly of simple and complex carbides surrounded by an iron based solid solution phase which is preferentially dissoluted in most of the electrolytes used in the tests. The passivation ability was studied in electrolytes with various pH values ranging from 0 to 14. When compared with the bulk glassy alloy, the crystalline counterpart is less noble in all the electrolytes, but exhibits no significant difference in the anodic polarization behaviour. Both of them exhibit low corrosion current densities in the whole pH value range ($<3\ \mu A/cm^2$). The passivation ability is very poor in strongly acidic solutions and improves with increasing pH, being the best at pH 11. Passive films on the glassy sample were characterized by Auger electron spectroscopy. They are composed mainly of Fe and Cr oxides. Passivity greatly depends on the electrolyte composition: sulphates, as well as chlorides worsen the passive film protective character. Still, at room temperature, chloride concentrations up to 1 M do not bring about pitting. The influence of the alloy composition on passivity is discussed.

MM 48: Nanostructured Materials IV

Time: Friday 10:15–12:00 Location: IFW B

MM 48.1 Fri 10:15 IFW B

'Non-Equilibrium' Grain Boundaries in Severely Deformed Materials: Myths vs. Reality — •Sergiy Divinski and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Germany

Recent results on radiotracer diffusion in nanostructured and ultrafine grained materials produced by severe plastic deformation are reviewed. The data reveal a strong hierarchy of short-circuit diffusion paths in these materials – the ultra-fast diffusion paths (the top level of the hierarchy) turn out to be embedded in a network of relatively slower diffusion paths (the bottom level). The 'slow' paths are shown to represent the relaxed high-angle grain boundaries, which are the fastest short-circuit diffusion paths in annealed coarse-grained counterparts. The nature and origin of the ultra fast paths is examined and discussed in relation to the so-called "non-equilibrium"grain boundaries in severely deformed materials.

MM 48.2 Fri 10:30 IFW B

Ultra-fast diffusion pathways in severely deformed Nickel — •Gerrit Reglitz[1], Yuri Estrin[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Germany — [2]Monash University, Claytoon, Victoria, Australia

During recent years, so-called non-equilibrium grain boundaries with high densities of extrinsic (excess) dislocations have been suggested to exist in severely deformed materials. These defects that are supposedly characterized by a large excess energy density are brought forward in explanations of the unusual properties and property combinations of such materials. However, such grain boundaries should also present highly unusual diffusion properties, i.e. the grain boundary diffusivity of non-equilibrium grain boundaries should be much higher than the diffusivity of conventional high-angle grain boundaries.

In order to analyze the possible existence of these non-equilibrium defects, grain boundary diffusion studies on Ni after severe plastic deformation by Equal Channel Angular Pressing has been carried out by applying the ^{63}Ni radioisotope in combination with the parallel sectioning technique. First results indicate the existence of ultra fast short-circuit diffusion parts with duffusivities of several orders of magnitude higher than the diffusivities of relaxed high-angle grain boundaries. These results together with recent results obtained on pure Cu and Cu-rich alloys deformed also by ECAP are discussed with respect of the origin of these ultra-fast diffusion pathways and their possible relation to non-equilibrium grain boundaries.

MM 48.3 Fri 10:45 IFW B

Annealing behaviour of equiatomic nanocrystalline NiTi alloy produced by high-pressure torsion — •Reeti Singh[1], Sergiy Divinsky[1], Ruslan Z. Valiev[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wihelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149, Münster, Germany — [2]Institute of Physics of Advance Materials, Ufa State Aviation University,12 K. Marx Street, 450000 Ufa, Russian Federation

A nanocrystalline $Ni_{50}Ti_{50}$ alloy that had been severely deformed by high-pressure torsion (HPT) was investigated. Both amorphous and nanocrystalline phases were found to co-exist in the as-prepared state. Crystallization and structural changes during annealing were investigated by differential scanning calorimetry (DSC), X-ray diffraction analysis and transmission electron microscopy.

The DSC thermograms and X-ray analyses reveal stress relaxation and partial crystallization below 500 K while grain growth of the nanocrystals occurs predominantly after heating to temperatures above 523 K. The activation energy of grain growth was estimated to be 289 kJ/mole by applying a Kissinger analysis. Along with the amorphous phase crystallization, a continuous growth of pre-existing nanocrystals that are retained after HPT, is observed. The DSC signals observed during continuous heating experiments indicate an unusually large separation between the nucleation and the growth stages. This behavior, that also causes a large variation of the nanocrystal size after annealing at higher temperatures, is discussed with respect to the nanoscale microstructural heterogeneity after initial deformation.

MM 48.4 Fri 11:00 IFW B

Microstructure and texture evolution during high pressure torsion of a Cu-0.17wt%Zr alloy — •Anahita Khorashadizadeh, Myrjam Winning, and Dierk Raabe — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Investigations of the microstructure of materials processed via severe plastic deformation methods such as high pressure torsion and their recrystallization behavior is of great interest as they are capable of producing ultra fine grained material with good mechanical properties. In this study Cu-0.17wt%Zr has been subjected to high pressure torsion (HPT) with a maximal pressure of 4.8 GPa at room temperature up to shear strains of γ=78. Annealing of the deformed samples was carried out subsequently and microstructure of both the deformed and annealed samples was investigated using a scanning electron microscope and microhardness measurements, in order to analyze the recrystallization behavior of the HPT samples. It will be shown that simple shear texture components represented by A-fiber {111}<uvw> and B-fiber {hkl}<110> were developed during the HPT deformation. After annealing, the ideal shear texture components still exist despite a change in texture intensity. The local orientations of deformed and annealed samples were analyzed using electron back scatter diffraction to obtain information about the recrystallization process.

MM 48.5 Fri 11:15 IFW B

Mechanical Properties of Nanocrystalline Palladium Prepared by Magnetron Sputtering — •Anna Castrup[1,2], Torsten Scherer[1], Yulia Ivanisenko[1], Horst Hahn[1,2], In-Suk Choi[1], and Oliver Kraft[1] — [1]Forschungszentrum Kalrsruhe, Germany — [2]Technical University of Darmstadt, Germany

Nanocrystalline metals and alloys with grain sizes well below 100 nm often demonstrate unique deformation behaviour and therefore attract a great interest in material science. The understanding of deformation mechanisms operating in nanocrystalline materials is important to predict their mechanical properties.

In the present study Pd films of 1 μm thickness were prepared using UHV rf magnetron sputtering on dog bone shaped Kapton substrates and on Si/SiO2 wafers. The films were sputtered using multilayer technology with an individual layer thickness of 10 nm. This resulted in grain sizes of about 20 nm.

Initial microstructure and texture were characterized using conventional XRD measurements and transmission electron microscopy (TEM) in both cross section- and plane view. The mechanical properties were investigated using tensile testing and nanoindentation at several strain rates. An increased hardness and strength as compared to coarse grained Pd was observed, as well as high strain rate sensitivity. The microstructure in the gauge section after tensile testing was again analyzed using TEM in order to reveal signatures of deformation mechanisms like dislocation motion or twinning.

MM 48.6 Fri 11:30 IFW B

Plasticity in Nanocrystalline Tungsten — •Jonathan Schäfer and Karsten Albe — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

Computational simulation methods such as the molecular dynamics method are very useful to gain more insights into the deformation mechanisms of nanocrystalline materials. Especially for the class of fcc metals a lot of simulations have been carried out in the past in order to investigate dislocation emission, grain boundary sliding, and other processes on the atomic level. For the class of bcc materials, however, a complete map of deformation mechanisms is still missing and supposed mechanisms like the formation of cracks at the grain boundaries have not been confirmed yet. Tungsten as a bcc model material is of particular interest because its melting point, which is higher than for any fcc material, might permit the observation of thermally activated processes during deformation at elevated temperatures. We present Molecular Dynamics simulations of nanocrystalline Tungsten model structures generated using the Voronoi method. Deformation experiments are carried out at different temperatures and various loading conditions. The role of the interatomic potential (Analytic bond order potential, Finnis-Sinclair potential) and the influence of the structure synthesis method on the mechanical behavior are assessed. Additionally, mechanisms like crack formation at grain boundaries are addressed.

MM 48.7 Fri 11:45 IFW B

Microstructure, texture and mechanical properties of ultrafine-grained Al alloys produced by accumulative roll bonding — •Juliane Scharnweber[1], Werner Skrotzki[1], Carl-Georg Oertel[1], Heinz-Günter Brokmeier[2], Heinz Werner Höppel[3], and Irena Topic[3] — [1]Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden — [2]GKSS Forschungszentrum, 21494 Geesthacht — [3]Lehrstuhl Allgemeine Werkstoffwissenschaften, Universität Erlangen-Nürnberg, 91058 Erlangen

The microstructure and local texture of ultrafine-grained Al alloys produced by accumulative roll bonding (ARB) up to 8 cycles were determined by electron backscatter diffraction (EBSD) mapping. The local textures within the thickness of the sheet will be compared with global textures measured by neutron diffraction. Additionally, tensile tests at constant strain rate were applied at room temperature. The strength increases while the ductility of about 4% is independent of the number of ARB cycles. Based on the experimental results the evolution of the microstructure during the ARB process and its kinetics will be discussed.

MM 49: Hydrogen in Metals

Time: Friday 10:15–11:45 Location: IFW D

MM 49.1 Fri 10:15 IFW D

Universal trends for the solubility of hydrogen in non-magnetic 3d transition metals derived from first principles — •Ugur Aydin, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung

Hydrogen is an omnipresent element in many materials which may cause materials failure (e.g. hydrogen embrittlement) or maybe used for hydrogen storage. Therefore a detailed understanding/prediction of H solubility (energetics) and kinetics in metals is crucial. In order to identify chemical trends for the solubility and mobility of hydrogen in metals we have performed an extensive ab initio study. Since the number of valence electrons was supposed to have a decisive influence on the quantity, the complete set of all 3d transition metals has been studied under comparable conditions (pure elements, no magnetism, identical fcc lattice structure). With respect to the site preference of the hydrogen atom in these metals, we have identified two different classes, with either the octahedral or the tetrahedral interstitial site being preferred. The corresponding H solution enthalpies, calculated for different lattice constants of the host metal, revealed a remarkable universal trend for all elements. The universal curve has a minimum formation energy (i.e. maximum hydrogen solubility) at a critical fcc lattice constant of ≈ 4.6 Å. Analyzing the data we find that the shape of the curve is a consequence of a volume dependent contribution and the specific electronic configuration of the host material. Based on these results we discuss strategies to identify systems with a optimum H solubility.

MM 49.2 Fri 10:30 IFW D

Hydrogenation Behaviour of Titanium Thin Films — •Ervin Tal-Gutelmacher, Ryota Gemma, Astrid Pundt, and Reiner Kirchheim — Institute for Materials Physics, University of Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen

Titanium films of different thicknesses were prepared on sapphire substrates in an UHV chamber, by means of ion beam sputter deposition under Ar-atmosphere at the pressure of 1,5*10E-4 mbar. For electrochemical hydrogen loading, the films were covered by a 30 nm thick layer of Pd in order to prevent oxidation and facilitate hydrogen absorption. In-situ stress measurements were conducted during step-by-step electrochemical hydrogen charging of the films. XRD measurements using a Phillips X-Pert diffractometer with a Co-Kα radiation were performed before and after hydrogenation in order to investigate the effect of hydrogen loading on the microstructure. The phase boundaries, as well as the stress and strain development during hydrogen absorption, depend strongly on the crystallographic growth orientation of the films. The main characteristics of absorption behaviour of hydrogen, as well as the thermodynamics and phase boundaries of titanium-hydrogen thin films are discussed in detail with specific emphasis on the comparison to titanium-hydrogen bulk system. Shifted grain boundaries and narrowed two-phase field appear in Ti-H film system, which are mainly attributed to the microstructural contribution, as well as to the large stresses in the GPa-range that built up between the films and their substrate.

MM 49.3 Fri 10:45 IFW D

Quantitative determination of the hydrogen in zirconium with high spatial resolution by means of neutron radiography — •Mirco Grosse — Forschungszentrum Karlsruhe, Germany

Due to the high total neutron cross section of hydrogen, neutron radiography is a powerful tool for quantitative hydrogen determination in a lot of materials with a spatial resolution up to 0.030 mm.

As example, studies of the hydrogen uptake during steam oxidation of zirconium based alloys applied as nuclear fuel cladding materials are given.

Correlation parameters between the total neutron cross section of the sample and its hydrogen content were determined. At H/Zr atomic ratios lower than 1.0, linear correlations between the hydrogen content and total cross section exist. The total cross section of Zr is lower and the effect of the hydrogen is higher in radiography measurements with a cold neutron spectrum than with a thermal spectrum.

After an initial phase a dynamical equilibrium is established between the hydrogen released into the gas phase and absorbed into the remaining metal. Due to the parabolic oxidation kinetics the hydrogen concentration decreases by the power of -1/4 with time.

The method provides also the possibility of in-situ measurements. Examples for the hydrogen uptake during isothermal steam oxidation will be given.

MM 49.4 Fri 11:00 IFW D

A multiscale study of hydrogen embrittlement in metals: The hydrogen enhanced local plasticity (HELP) mechanism — •Johann von Pezold and Jörg Neugebauer — Max Planck Institut für Eisenforschung GmbH, Düsseldorf, Germany

The embrittlement of metals by H is a long-standing problem, whose underlying mechanisms are still largely unclear. In this study we consider the atomistic basis of the HELP mechanism, which asserts that H mobilises dislocations by shielding elastic dislocation-dislocation and dislocation-solute interactions.

Using a combination of density-functional theory calculations, semiempirical EAM potentials and an effective lattice gas Hamiltonian we determine the effect of H on the stress field around edge dislocations in fcc metals. The density of the H distribution around the dislocation core is determined by the H-H interaction: weak H-H interactions give rise to a dilute H distribution, while attractive H-H interactions entail a dense H distribution. The stress field around the dislocation in the presence of a dilute and a dense H distribution is used to critically discuss the H-induced shielding effect postulated by the HELP mechanism.

MM 49.5 Fri 11:15 IFW D

Atom probe tomography analyses of deuterium distribution in Fe/V multi-layered films — •Ryota Gemma, Talaat Al-Kassab, Reiner Kirchheim, and Astrid Pundt — Institut fuer Materialphysik, Friedrich-Hund-Platz 1, D-37077, Goettingen, Germany

Recently, the interaction of hydrogen with metallic multi-layered thin films remains as a hot topic. A detailed knowledge on such chemically modulated systems is required if they are desired for application in hydrogen energy system as storage media. In this study, the deuterium (D) concentration profile of Fe/V multi-layer was investigated by atom probe tomography (APT) between 60 and 20 K. It is firstly shown that a deuterium-loaded sample can easily react with oxygen at Pd capping layer on Fe/V and therefore, it is required to avoid any oxygen exposure after D_2 loading before APT analysis. The analysis temperature also has an impact on the D concentration profile. The results taken at 60 K show clear traces of surface segregation of D atoms diffusing towards the analysis surface. The observed diffusion profile of D regarding analysis time allows us to estimate an apparent diffusion coefficient. The calculated diffusion coefficient at 60 K is in the order of 10^{-17}cm^2/s which deviates about 6 orders of magnitude from a value extrapolated from high temperatures. Below 30 K, the D concentration profile shows no segregation anymore and a

homogeneous distribution with $c_D = 0.05(2)$ D/Me, which is in good accordance with that measured in corresponding pressure-composition isotherm of H-Fe/V system.

MM 49.6 Fri 11:30 IFW D

Study of complex hydrides prepared by mechano-chemical synthesis — •Carine Rongeat, Christian Geipel, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

Ball milling has been widely used for the synthesis of metal hydrides, e.g. MgH2, with high sorption performances. However, metal hydrides cannot address the requirements imposed for solid state hydrogen storage in mobile application. A new class of hydrides, the complex hydrides are attracting much interest due to their high capacity and predicted moderate temperature of operation. High-pressure reactive milling with in-situ monitoring the pressure and temperature was applied to the synthesis of NaAlH4 doped with different additives. Useful information on the kinetic properties of the compound could be derived from this system already during synthesis. The same system was applied for the synthesis of Ca(BH4)2 but different results were obtained due to the higher stability of the boride compounds used. Finally, another route for the synthesis of complex hydride is to performed the metathesis reaction during milling, e.g. the synthesis of Mg(BH4)2 can be obtained (with LiCl) by the reaction between LiBH4 and MgCl2. All the compounds synthesized by mechano-chemical synthesis are analyzed by means of advanced structural characterization techniques (Raman spectroscopy, XPS, in-situ XRD). Their hydrogen sorption properties were also studied by various methods (DSC, TGA).